National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

William Thigpen
NASA Advanced Supercomputing Division

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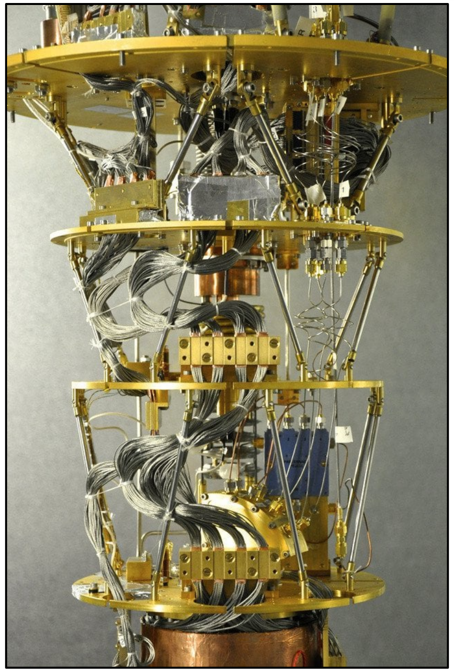
Quantum Computing Prototyping Environment Deployed

- The HECC Cloud team deployed a Quantum Computing environment that provides access to multiple quantum computing machines in Amazon Web Services (AWS).
- The team forged an agreement with NASA’s Enterprise Managed Cloud Computing (EMCC) team to create the sandbox environment.
- A select researcher was able to use a web-based notebook interface to access quantum computers through the AWS BraKet application programming interface.
  - The environment includes Kubernetes-based scaling for non-quantum tasks and long-term file storage.
- Several quantum computing systems from Rigetti, IonQ, Oxford Quantum Circuits, Xanadu, and QuEra were made available for the researcher to experiment with.
- The HECC Cloud team is working on transitioning the environment from an EMCC sandbox to an operational environment for future HECC users.

IMPACT: Enabling HECC users to experiment with different quantum hardware and begin exploratory work with these low technology readiness level (TRL) quantum computing devices is critical to advancing forward into one of the new computing paradigms needed to meet NASA’s mission requirements.



Dilution refrigerator in a D-Wave Two quantum computer.
John Hardman, NASA/Ames

Pathfinding AMD Instinct MI210 GPU Testbed Installed

- To evaluate alternative architectures for future HPC needs, HECC systems and applications experts recently installed a two-node AMD MI210 testbed system. The system was installed as part of a pathfinding infrastructure project.
  - Each node is equipped with one AMD EPYC 7763 64-core processor and four AMD Instinct MI210 GPUs. Each node has 256 GB of host memory, and each MI210 GPU has 64 GB of high-bandwidth memory.
  - The Systems teams installed the TOSS4 (RHEL 8.7) operating system, PBS 21.1c job scheduler, and AMD ROCm software stack.
- The Application Performance and Productivity (APP) team assisted and verified that required software for building and running GPU applications on the system was correctly installed. The team:
  - Verified the use of the AMD Heterogeneous Interface for Portability (HIP) and ROCM math libraries.
  - Built and ran a “HIPifyed” version of the CATMIP application.
  - Confirmed the setup for successfully running multi-node jobs.
- The system is open for general user access. The APP team will conduct performance studies with more applications, including NAS Parallel Benchmarks and a lattice quantum chromodynamics application, and compare results with other types of GPUs such as the NVIDIA A100.

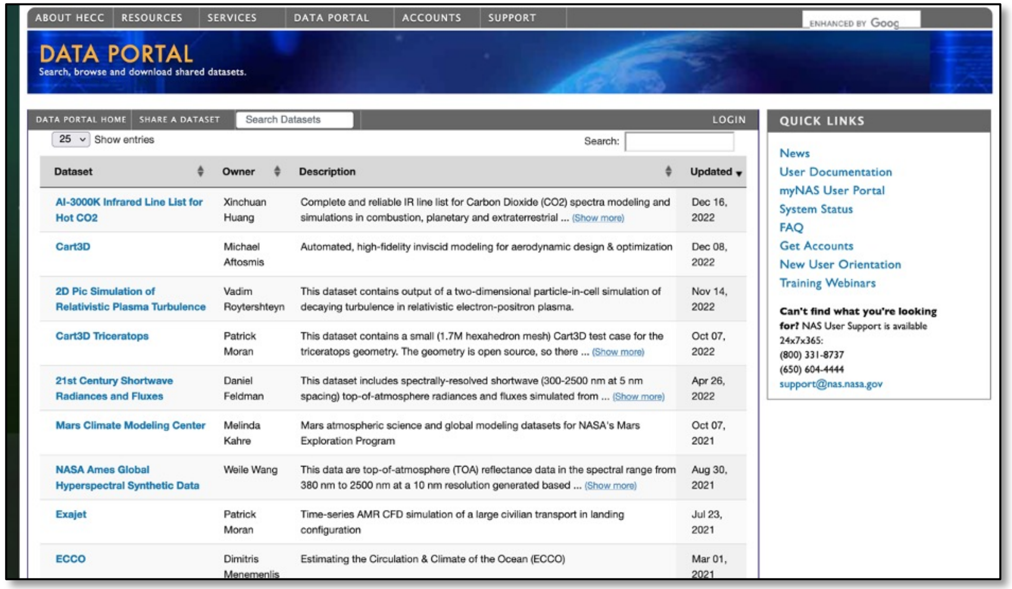
IMPACT: HECC’s evaluation of alternative architectures is critical for satisfying future NASA computing requirements. GPU-accelerated systems have the potential to lower the cost of computing for a significant portion of HECC resource workloads.

HECC installed a new AMD MI210 GPU-based system at the NASA Advanced Supercomputing facility as part of the pathfinding infrastructure project for evaluating future NASA needs.
Don Story, NASA/Ames

New Features Added to Data Portal

- HECC's Data Publication and Discovery team works closely with researchers to assist with data sharing and dissemination.
- The Data Portal home page was recently updated to accommodate the growing number of shared datasets.
  - Existing datasets can now be sorted by dataset name, data owner, or updated date.
  - Some of the datasets can also be examined using the new THREDDS data server to provide data in GeoTIFF and netCDF format, enabling users and collaborators to incorporate data into their workflows more efficiently.
  - Users can also search the information in the table of datasets.
- Users can specify a subset of a gridded datasets, gather metadata information, and/or visualize the extracted data through common scientific visualizing software packages. Through the Data Portal, large, multi-gigabyte datasets produced on HECC supercomputing resources can be easily accessed by science and engineering communities. These include: planetary science, e.g., Pluto and Titan climate modeling; Earth science, e.g., GeoNEX, carbon cycle, and ocean circulation; Heliophysics modeling and simulation; and aerospace modeling for design and optimization.

IMPACT: The Data Portal 's new features allow users to find datasets more quickly and easily and incorporate them into their workflows.

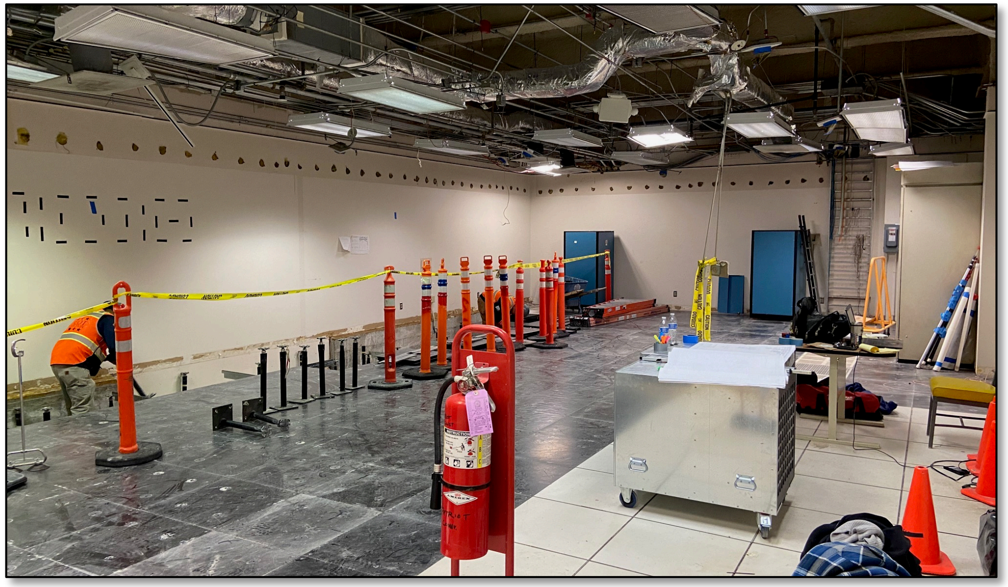


Screenshot of the Data Portal, which now supports multiple pages for a growing number of shared dataset listings. Since 2019, HECC has provided and maintained a central data portal where HECC users can upload raw or processed data to share with the public or with specified collaborators.

Construction for hyperwall Remodel Underway

- The hyperwall room in Building N258 is undergoing a remodel to develop it into a dedicated display viewing room. HECC and Ames Code J engineers, with contractor Patriot Construction, began construction in February.
- The room will accommodate a new, taller, and longer hyperwall display screen with over one billion pixels. Remodeling tasks include:
  - Remove hyperwall compute systems. The hyperwall-4 cluster, which replaced hyperwall-3, is now located in the main N258 computer room.
  - Remove the raised floor required by the hyperwall compute for cabling and cooling. Remove the computer room air handler and all supporting electrical infrastructure. Install new flooring on the concrete slab, which is two feet below the raised floor.
  - Remove the existing ceiling and fluorescent lighting. Install a new, higher ceiling and install new LED lights with lighting controls.
- Although the overall room dimension remain the same, the changes will enable researchers to explore their visualizations with new perspectives, and the enlarged viewing area will accommodate larger tours for NASA Ames demonstrations.

IMPACT: Modernizing and enlarging the hyperwall will enable higher definition visualizations and advance the scientific and aerospace community.

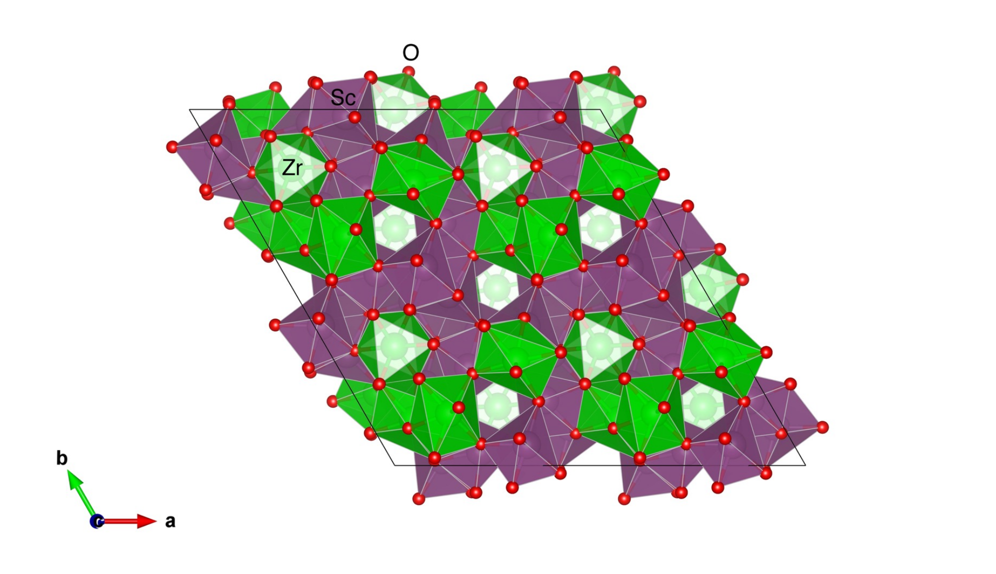


The hyperwall room at the NASA Advanced Supercomputing facility under construction; computers are already removed, ceiling and floor removal is underway. The power distribution units (blue) and air handler (beige, right) will also be removed.
Chris Tanner, NASA/Ames

A Quantum Mechanical Framework for Cosmochemistry and Materials Modeling*

- Researchers at the University of Arizona and NASA Kennedy Space Center used HECC resources to develop a new first-principles modeling framework that simulates materials starting from quantum-mechanical descriptions of atoms. These simulations require HPC to capture physics across vastly different length scales.
- The work supports NASA's study of the early solar nebula—which eventually evolved into our Solar System—as well as the agency's effort to design new alloys for oxygen production on the Moon.
- Using the model, the team predicted condensation sequences of refractory and ultra-refractory minerals within the high-temperature region of the early solar nebula. By simulating crystal chemistries in phases such as magnesium aluminate spinel, they developed a "nebular thermochronometer" to determine the temperatures of certain physical processes in the nebula.
- The team also predicted superior alloy compositions that can work at the extreme temperatures required for molten regolith electrolysis, the process NASA aims to use to produce oxygen from the lunar soil.

IMPACT: The new model plays a crucial role in several NASA projects, including a NASA Emerging Worlds cosmochemistry project to study the early solar nebula and the GaLORE project (Gaseous Lunar Oxygen from Regolith Electrolysis), which aims to achieve novel alloy design for oxygen production on the Moon.



A 456-atom supercell molecular structure of Allendeite ($Sc_4Zr_3O_{12}$), used to calculate phonons. The calculations are crucial to thermo-dynamic and kinetic modeling of meteoritic and ultra-refractory materials. *Venkateswara Rao Manga, University of Arizona*

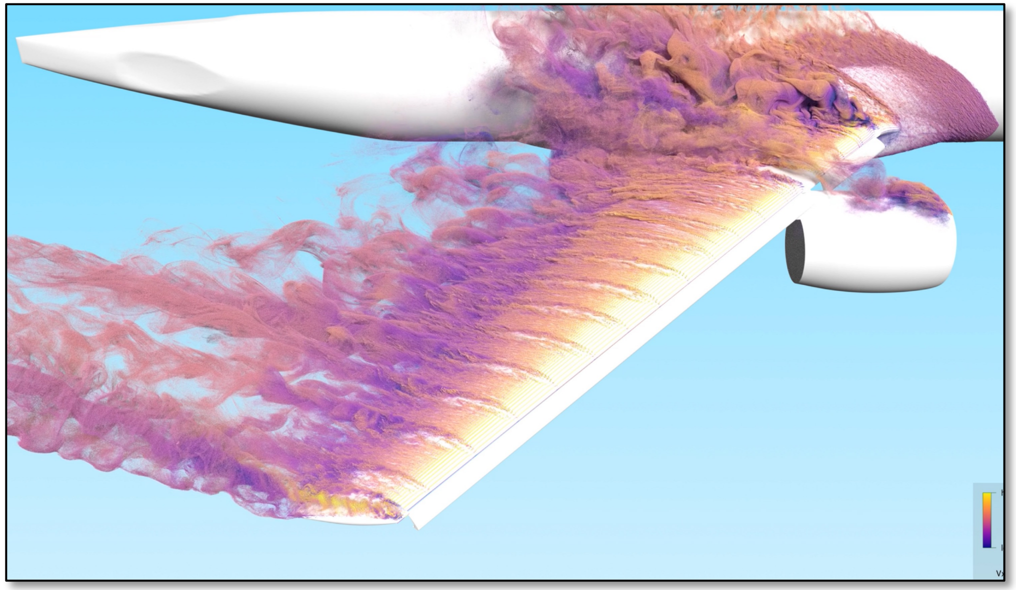
* *HECC provided supercomputing resources and services in support of this work.*

Computing WMLES for Aircraft Certification-by-Analysis*

- In order to accurately predict the notoriously challenging aerodynamics for aircraft with swept wings in high-lift configurations (take-off and landing), researchers in the NASA Advanced Supercomputing Division evaluated the current state-of-the-art computational fluid dynamics (CFD) tools to enable analysis-based compliance for aircraft certification.
- The Launch Ascent and Vehicle Aerodynamics (LAVA) team utilized two distinct technologies to compute high-lift wall-modeled large-eddy simulations (WMLES):
  - The first method used structured overset curvilinear grids, which are body aligned and can be carefully tailored for quality, but require intensive manual grid generation. More than two months of pre-processing time is needed to complete the required geometry.
  - The second method used fully automated structured octree-grids, which reduced the pre-processing time to roughly two hours of human effort, but produced less accurate geometries. To counter this, the team developed a new technique relying on immersed boundary closure.
- These simulations were the first to systematically show the qualitative nature of the convergence seen in pressure loading on high-lift geometries with grid refinement. The new, automated method increased computational affordability, drastically reduced pre-processing time, and provided computational predictions at a comparable accuracy-per-unit-cost to more complex methods.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: These technologies demonstrate the potential for further reduction in CFD simulation time, allowing NASA to use scale-resolving technologies for certification of future aerospace vehicles and missions.



Particle traces illustrating the flow topology on the suction side of the wing at an angle of attack of 21.5 degrees. The particle trajectories on the outboard part of the wing show the role of slat brackets/attachments at inducing separation on the outboard section, whereas strong corner flow separation is observed near the wing-body juncture. *Timothy Sandstrom, Gerrit Stich, NASA/Ames*

Papers

- "**V994 Herculis: A Unique Triply Eclipsing Sextuple Star System**," P. Zasche, et al., Monthly Notices of the Royal Astronomical Society, vol. 20, issue 2, published online January 31, 2023. *
  https://academic.oup.com/mnras/article-abstract/520/2/3127/7017852
- "**AI-3000K Infrared Line List for Hot CO_2**," X. Huang, et al., Journal of Molecular Spectroscopy, vol. 392, published online February 2, 2023. *
  https://www.sciencedirect.com/science/article/pii/S0022285223000139
- "**A Full Transit of ν^2 Lupi d and the Search for an Exomoon in its Hill Sphere with CHEOPS**," D. Ehrenreich, et al., arXiv:2302.01853 [astro-ph.EP], February 3, 2023. *
  https://arxiv.org/abs/2302.01853
- "**The Low Density, Hot Jupiter TOI-640 b is on a Polar Orbit**," E. Knudstrup, et al., arXiv:2302.01702 [astro-ph.EP], February 3, 2023. *
  https://arxiv.org/abs/2302.01702
- "**A Review of Common Natural Disasters as Analogs for Asteroid Impact Effects and Cascading Hazards**," T. Titus, et al., Natural Hazards, published online February 6, 2023. *
  https://link.springer.com/article/10.1007/s11069-022-05722-z
- "**Seasonal Forecasting Skill for the High Mountain Asia Region in the Goddard Earth Observing System**," E. Massoud, et al., Earth System Dynamics, vol. 14, issue 1, published online February 8, 2023. *
  https://esd.copernicus.org/articles/14/147/2023/

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- “**Searching for Gravitational-Wave Counterparts Using the Transiting Exoplanet Survey Satellite**,” G. Mo, et al., arXiv:2302.04881 [astro-ph.HE], February 9, 2023. *
  https://arxiv.org/abs/2302.04881
- ”**Numerical Investigation of Mach 2.5 Axisymmetric Turbulent Shock Wave Boundary Layer Interactions**,” J.-P. Mosele, et al., *Aerospace*, vol. 10, issue 2, February 9, 2023. *
  https://www.mdpi.com/2226-4310/10/2/159
- “**Temporal Albedo Variability in the Phase Curve of KELT-1b**,” H. Pariainen, Astronomy & Astrophysics, Letters to the Editor, vol. 671, published online February 9, 2023. *
  https://www.aanda.org/articles/aa/pdf/2023/03/aa45937-23.pdf
- “**TESS Discovery of Twin Planets near 2:1 Resonance around Early M Dwarf TOI 4342**,” E. Tey, et al., The Astronomical Journal, vol. 165, no. 3, published online February 9, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-3881/acaf88
- “**Simple, Fast Nitric Oxide Planar Laser-Induced Fluorescence Model for Computational Fluid Dynamics Applications**,” T. Drozda, et al., Journal of Aeronautics, published online February 12, 2023. *
  https://arc.aiaa.org/doi/full/10.2514/1.J062264
- “**A Second Earth-sized Planet in the Habitable Zone of the M Dwarf, TOI-700**,” E. Gilbert, et al., The Astrophysical Journal Letters, vol. 944, no. 2, published online February 16, 2023. *
  https://iopscience.iop.org/article/10.3847/2041-8213/acb599

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Papers (cont.)

- "**TOI-3235 b: A Transiting Giant Planet around an M4 Dwarf Star**," M. Hobson, et al., arXiv:2302.10008 [astro-ph.EP], February 20, 2023. *
https://arxiv.org/abs/2302.10008
- "**Recovering Thermodynamics from Spectral Profiles Observed by IRIS. (II). Improved Calculation of the Uncertainties Based on Monte Carlo Experiments**," A. Dalda, B. De Pontieu, The Astrophysical Journal, vol. 944, no. 118, February 20, 2023. *
https://iopscience.iop.org/article/10.3847/1538-4357/acb2c7/pdf
- "**A 2:1 Mean-Motion Resonance Super-Jovian Pair Revealed by TESS, FEROS, and HARPS**," V. Bozhilov, et al., arXiv:2302.10838 [astro-ph.EP], February 21, 2023. *
https://arxiv.org/abs/2302.10838
- "**Suppressing Quantum Errors by Scaling a Surface Code Logical Qubit**," Google Quantum AI, *Nature*, vol. 614, published online February 22, 2023. *
https://www.nature.com/articles/s41586-022-05434-1
- "**Introducing MPEC: Massively Parallel Electron Correlation**," D. Schwenke, Journal of Chemical Physics, vol. 158, issue 8, published online February 23, 2023.
https://aip.scitation.org/doi/full/10.1063/5.0135248
- "**On Improved Understanding of Airfoil Performance Evaluation Methods at Low Reynolds Numbers**," W. Koing, et al., Journal of Aircraft, published online February 27, 2023. *
https://arc.aiaa.org/doi/full/10.2514/1.C037023

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Presentations

- **NASA/Gulfstream Technical Interchanges Meeting**, Hampton, VA, February 7, 2023.
  - “**Advancements in Scale Resolving Simulations for High-Lift Predictions and Jet Aeroacoustics**,” J. Housman.
  - “**Sonic-Boom Predictions: Recent Enhancements to Cart3D**,” M. Nemec.
- “**NASA Focus on Sustainability and Reducing Impact on the Environment**,” W. Thigpen, Fujitsu ActivateNow Technology Summit, Silicon Valley, Mountain View, CA, February 9, 2023.
- **SIAM Conference on Computational Science and Engineering (CSE23)**, Amsterdam, February 26 – March 3, 2023.
  - “**Chemical Thermodynamics and the Mathematical Integration of Reaction Kinetics**,” A. Gouasmi.
  - “**Quantification of Numerical Uncertainty via Nonlinear Dynamical Approach**,” H. Yee.

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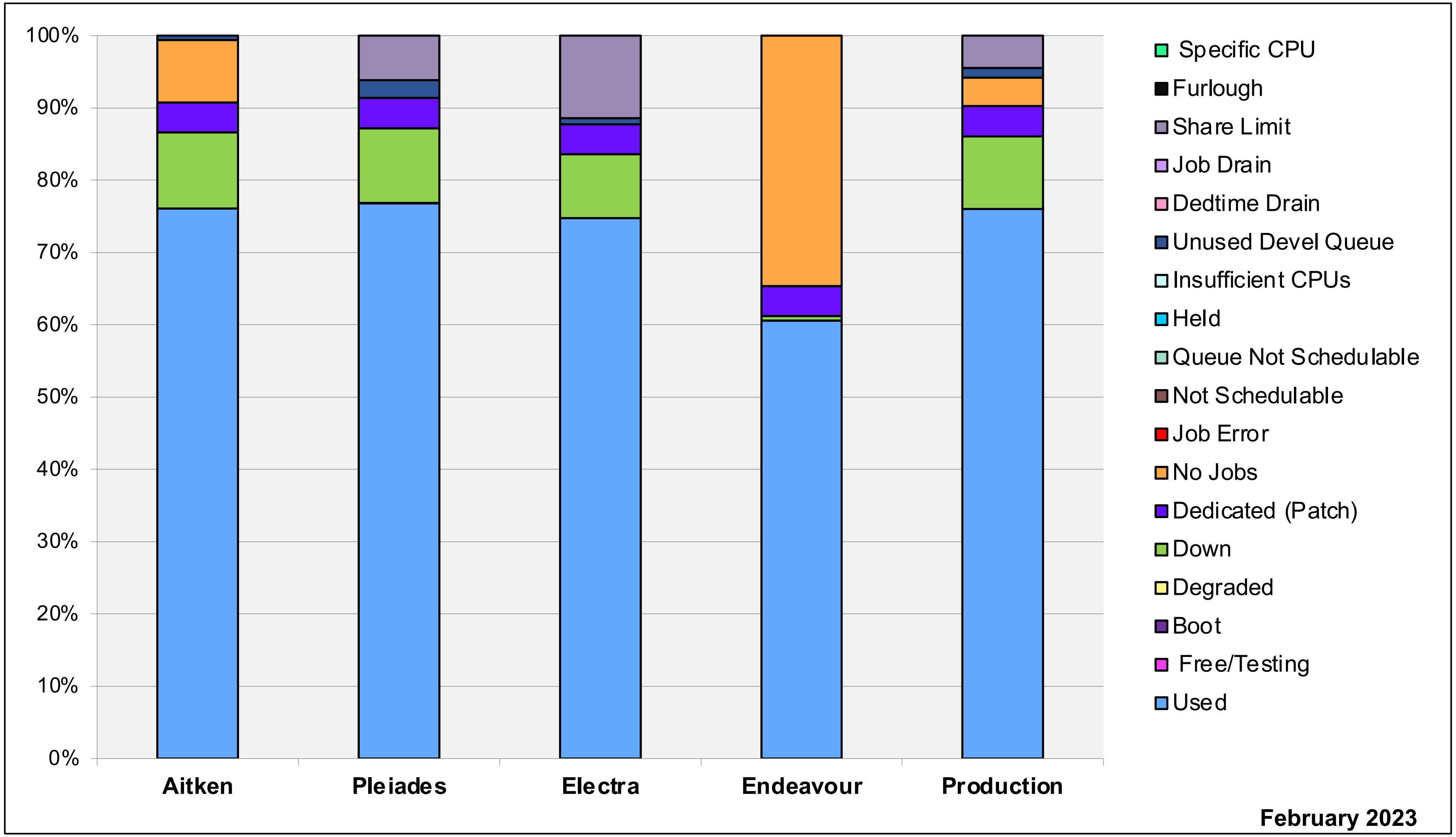
News and Events

- **Explaining a Solar Mystery – Princeton Researchers Have Discovered a Previously Hidden Heating Process**, *SciTech Daily*, February 4, 2023–Researchers discovered a previously unknown heating mechanism that explains why the solar corona, the atmosphere surrounding the Sun, is much hotter than the solar surface that emits it, using the largest turbulence simulations of their kind on HECC systems. *https://scitechdaily.com/explaining-a-solar-mystery-princeton-researchers-have-discovered-a-previously-hidden-heating-process/*

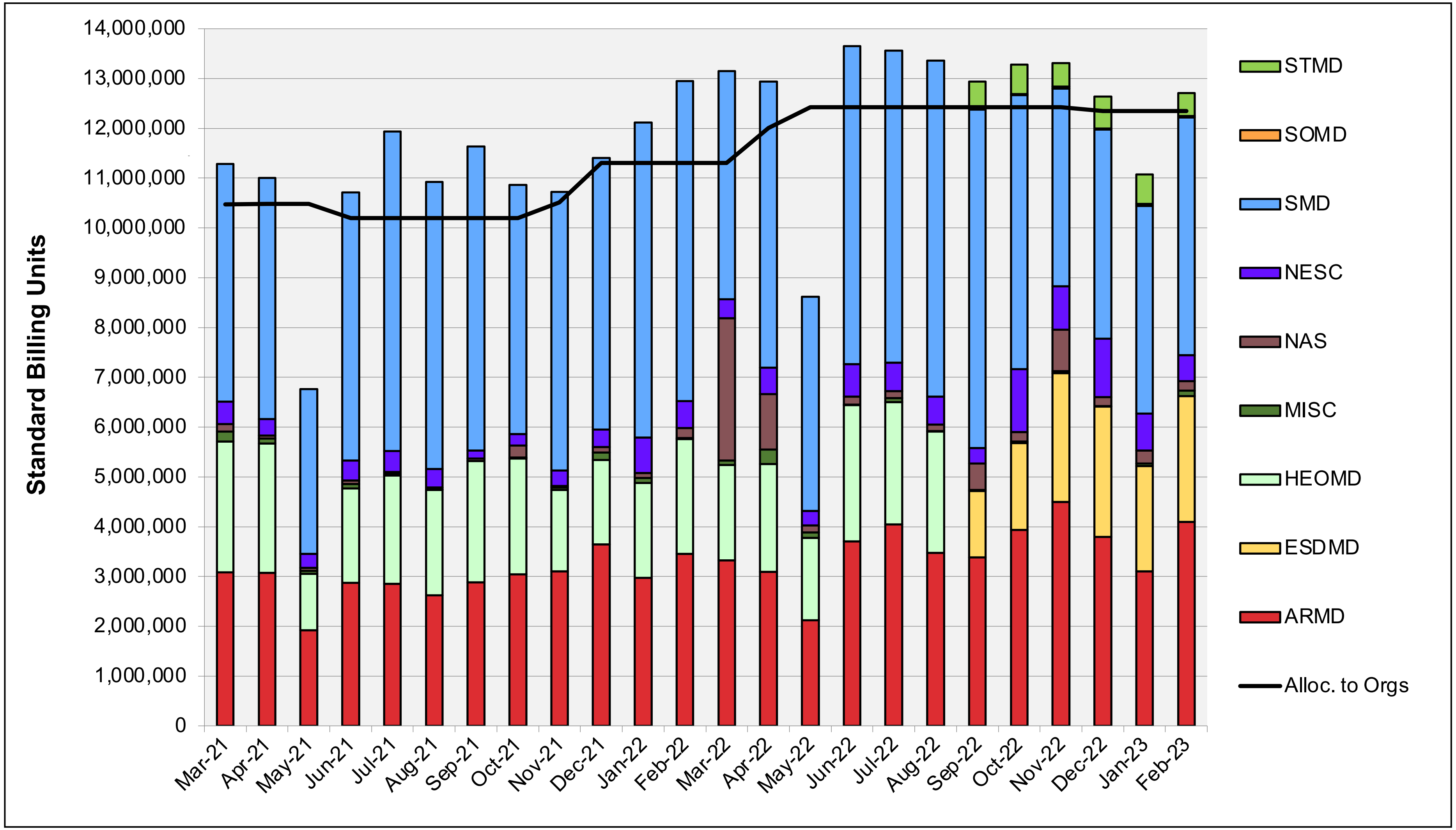
News and Events: Social Media

- **Coverage of NAS Stories**
  - Solar Flare/Sunquakes video:
    - NASA Supercomputing: Facebook 347 users reached, 10 reactions.
    - NAS: Twitter 1,876 views, 10 retweets, 23 likes.

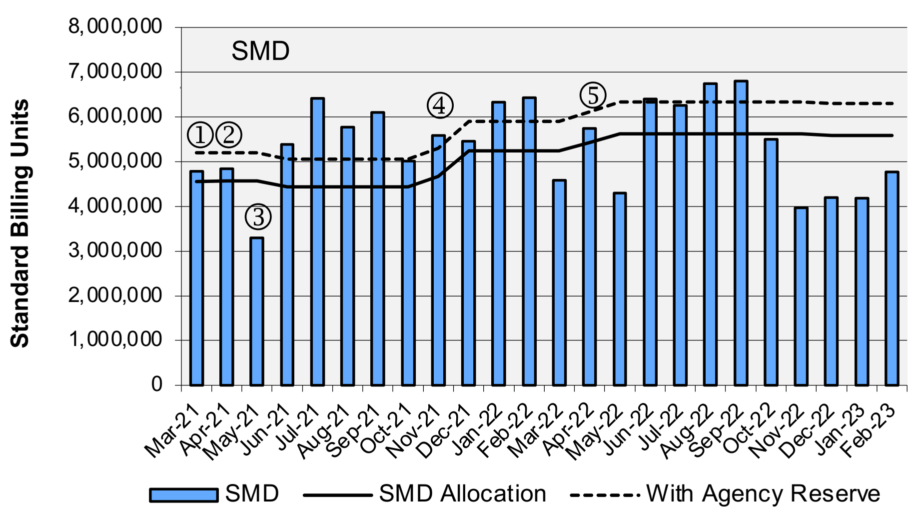
HECC Utilization

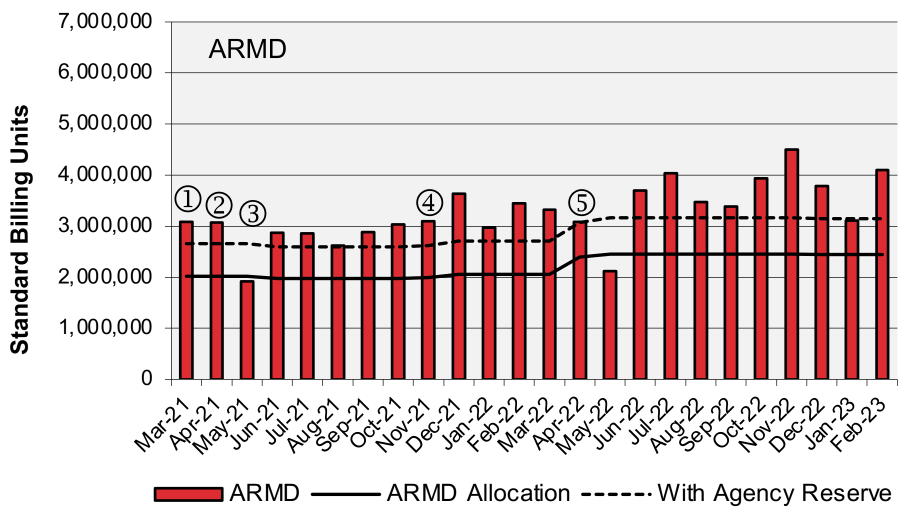


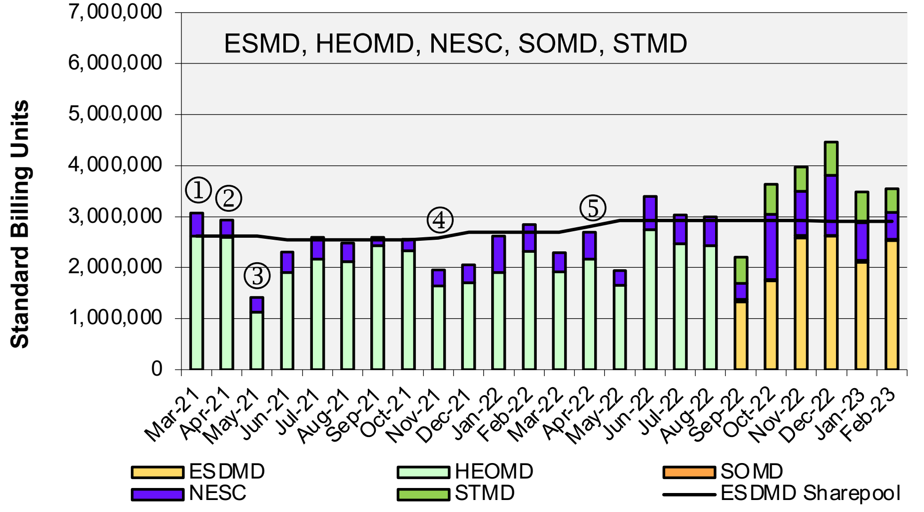
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 8 Rome Apollo racks introduced into Aitken

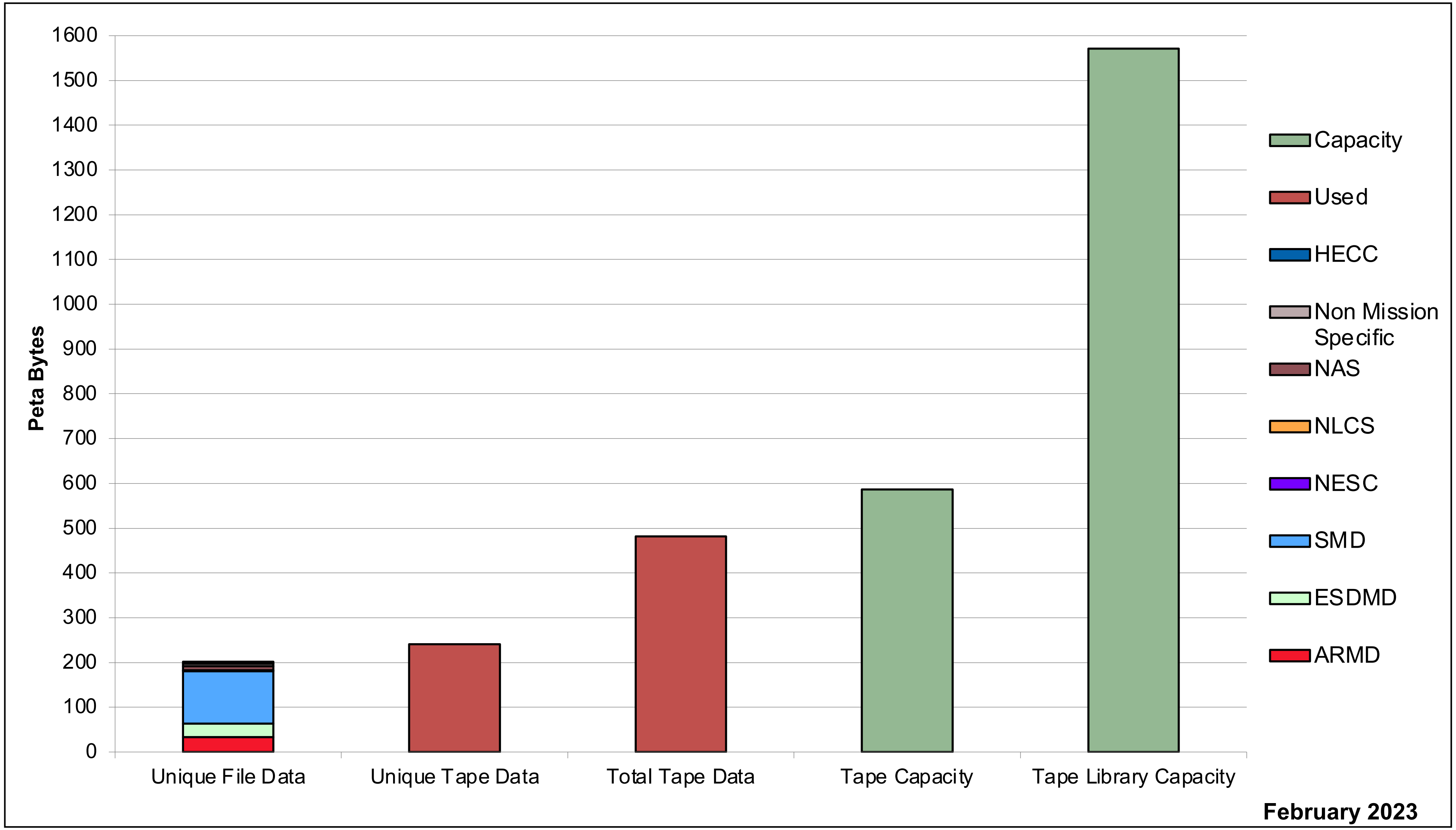
② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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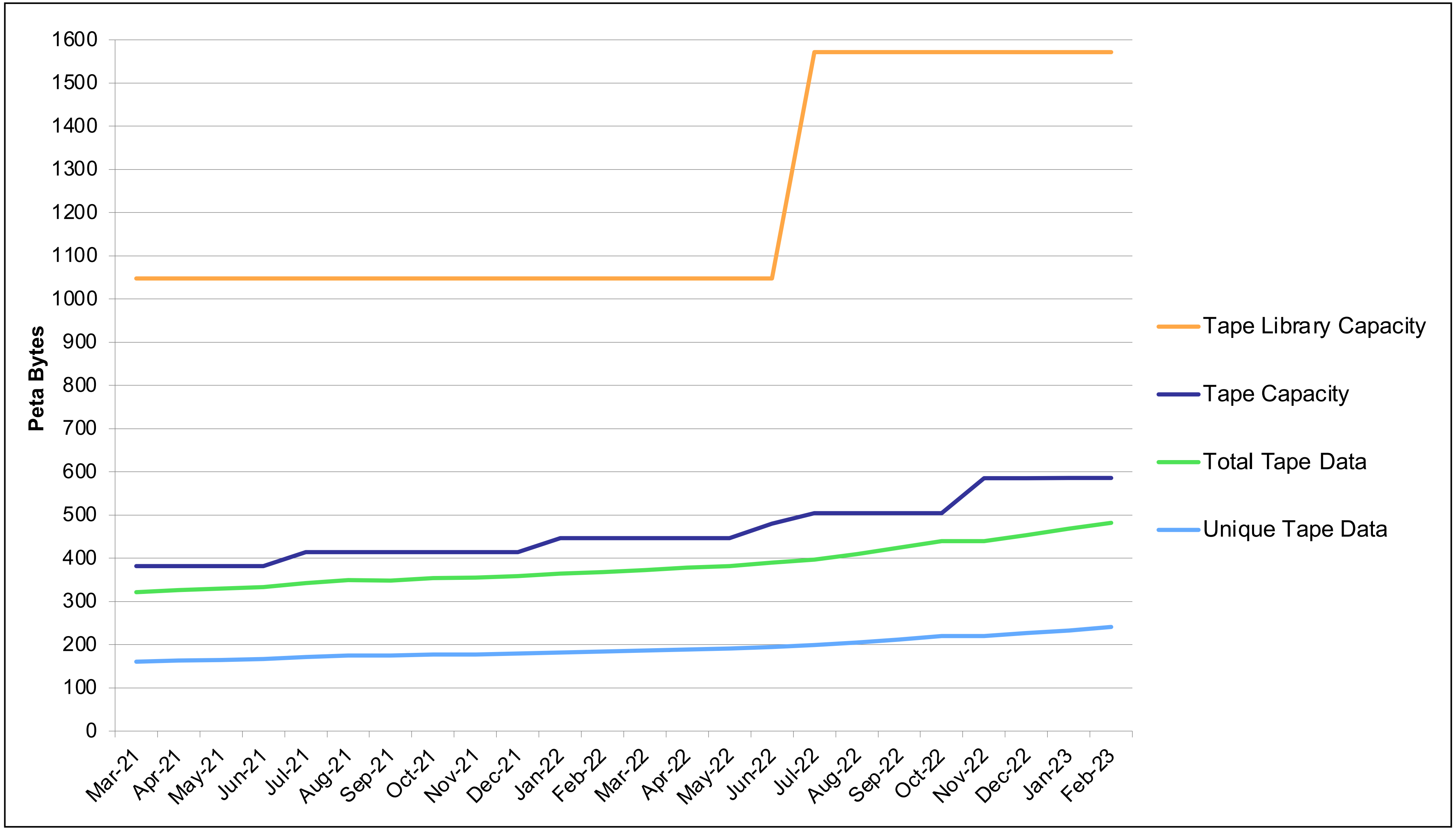
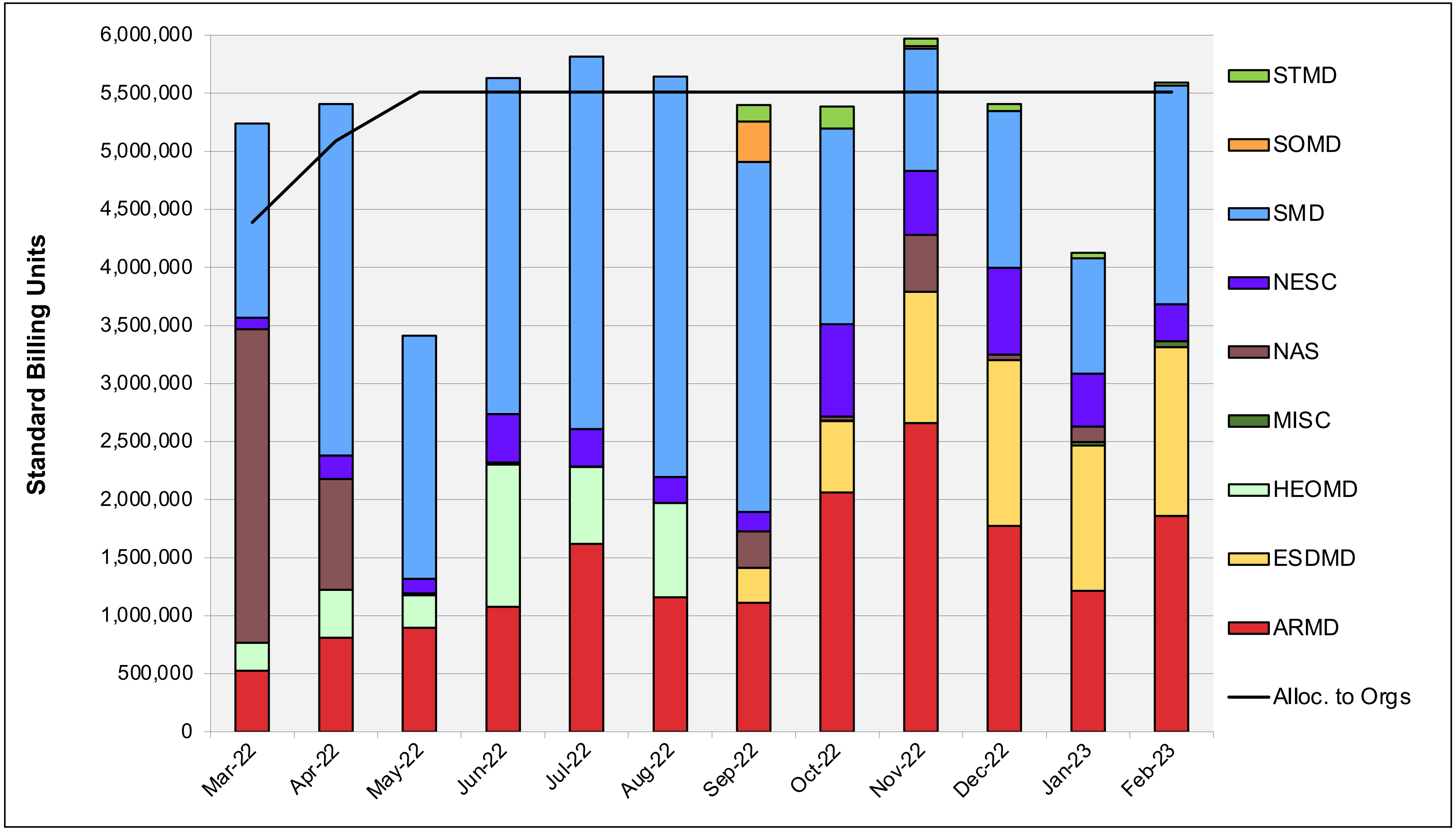
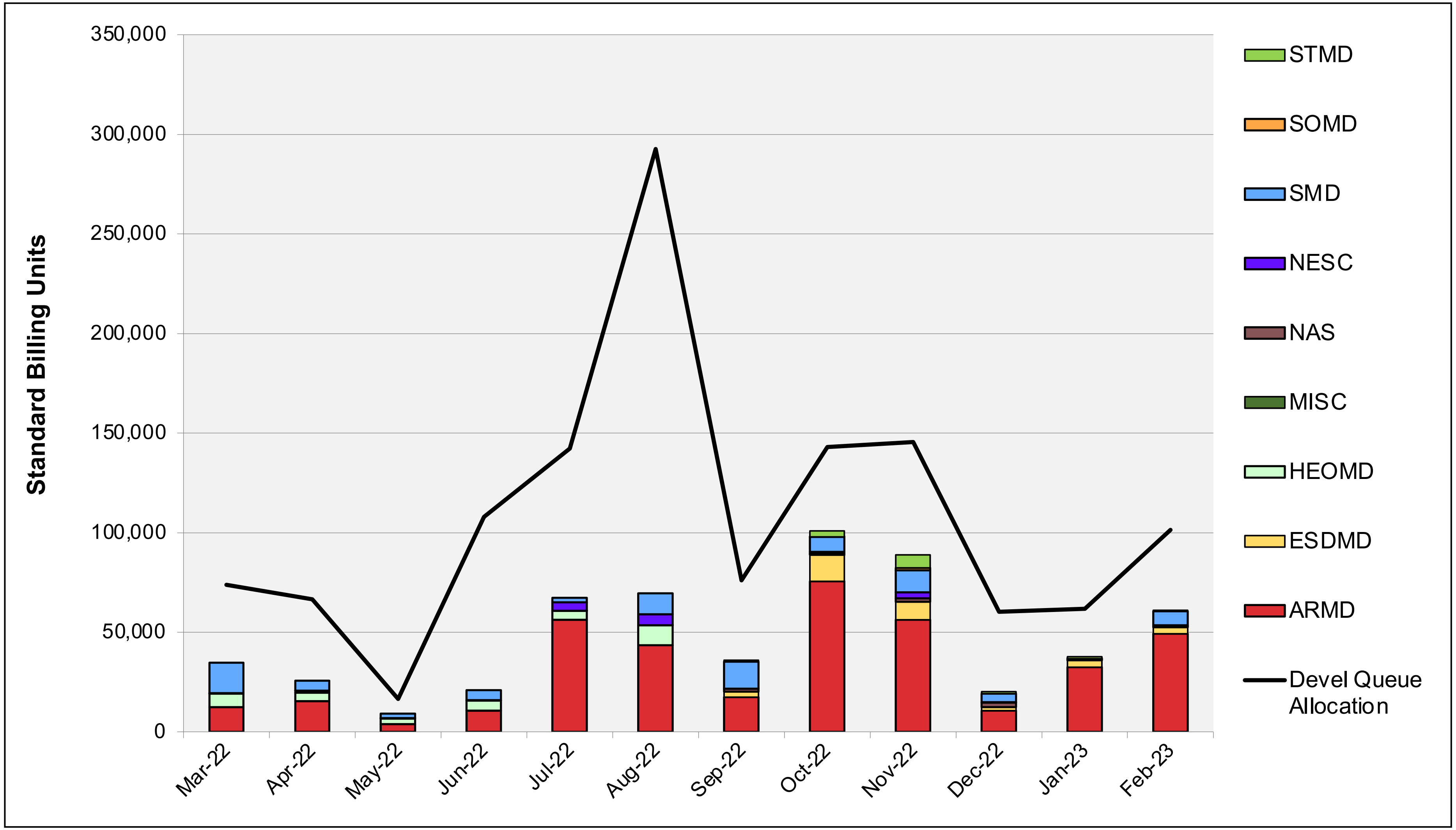


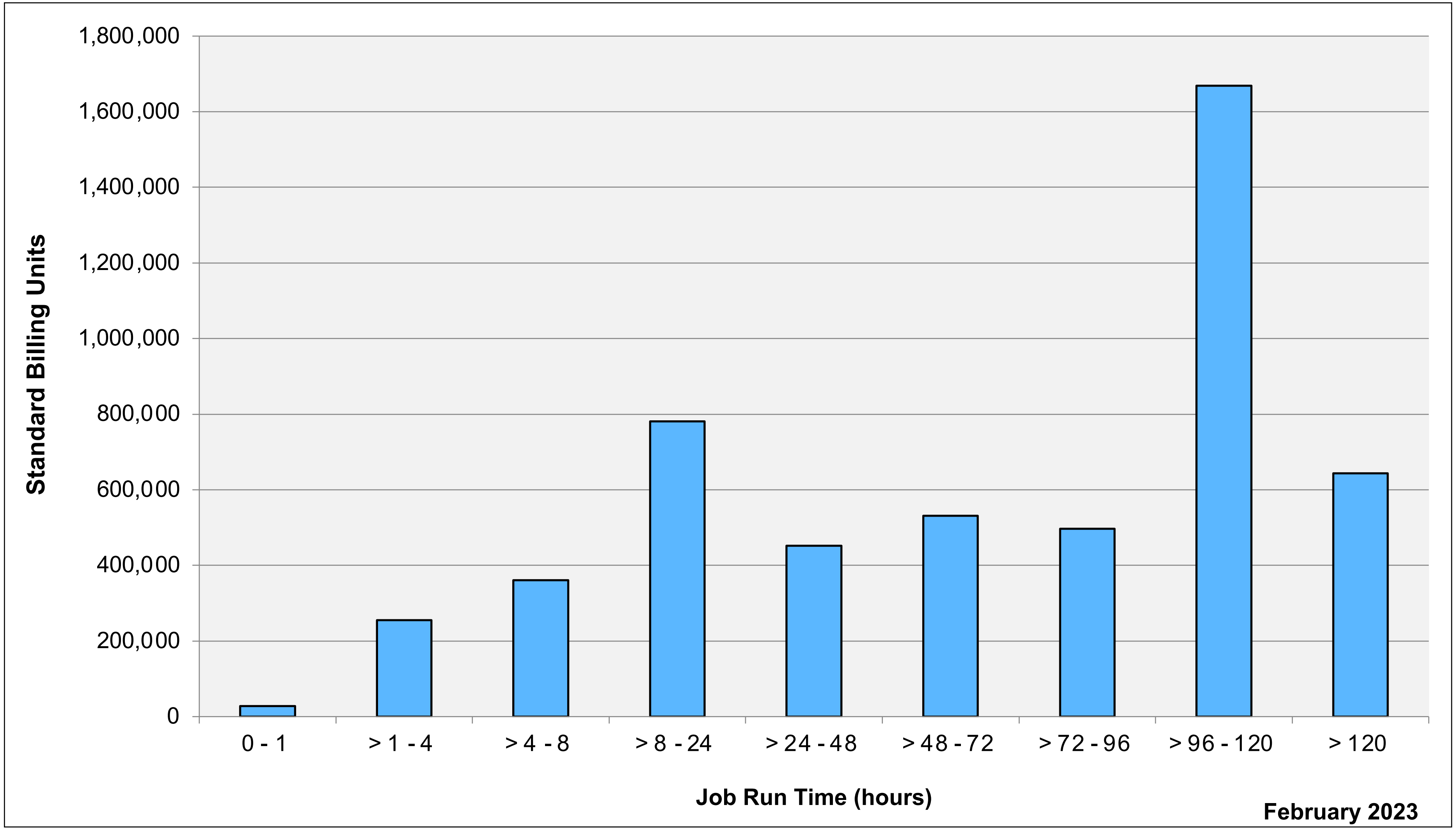
Aitken: SBUs Reported, Normalized to 30-Day Month



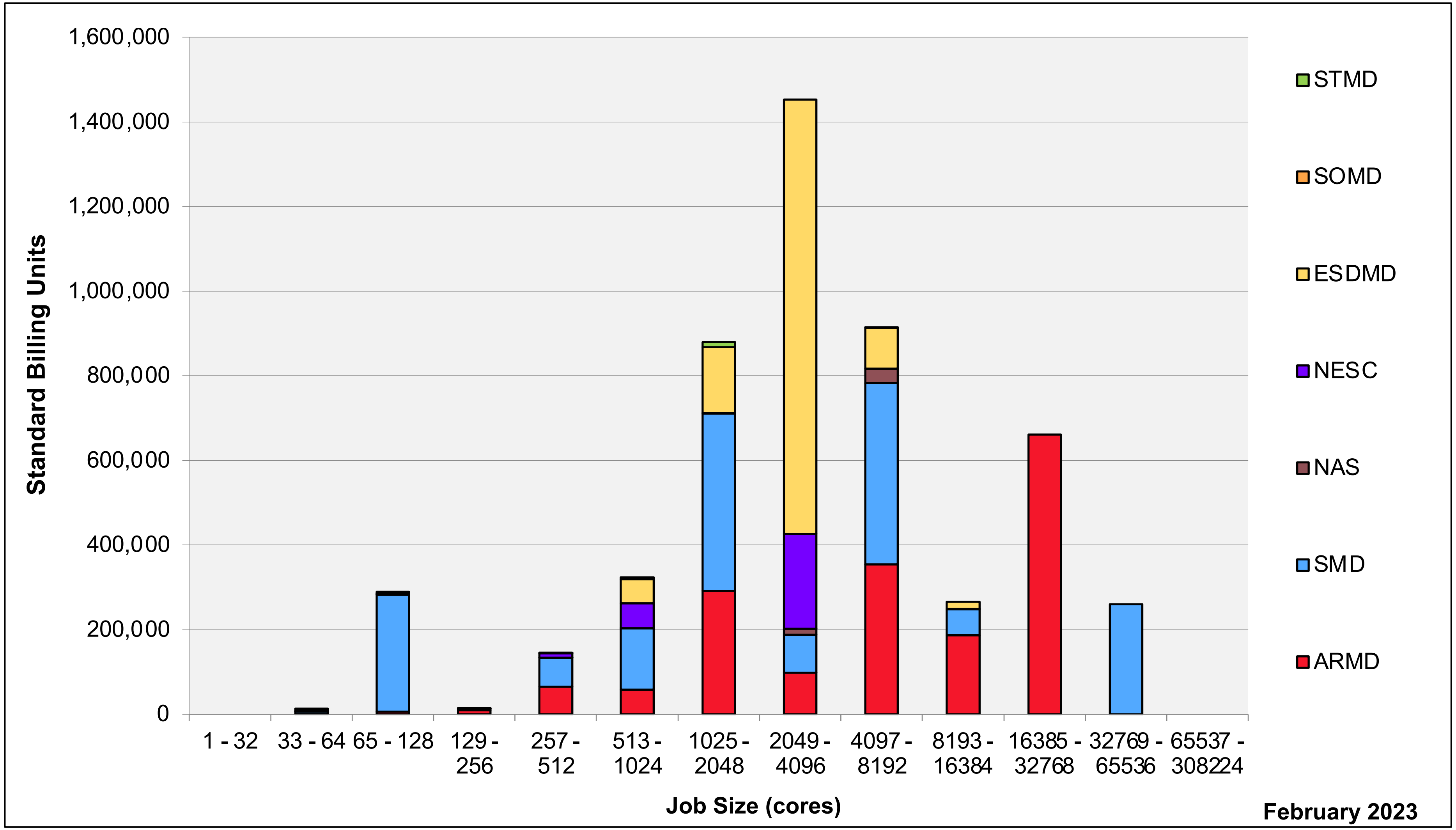
Aitken: Devel Queue Utilization



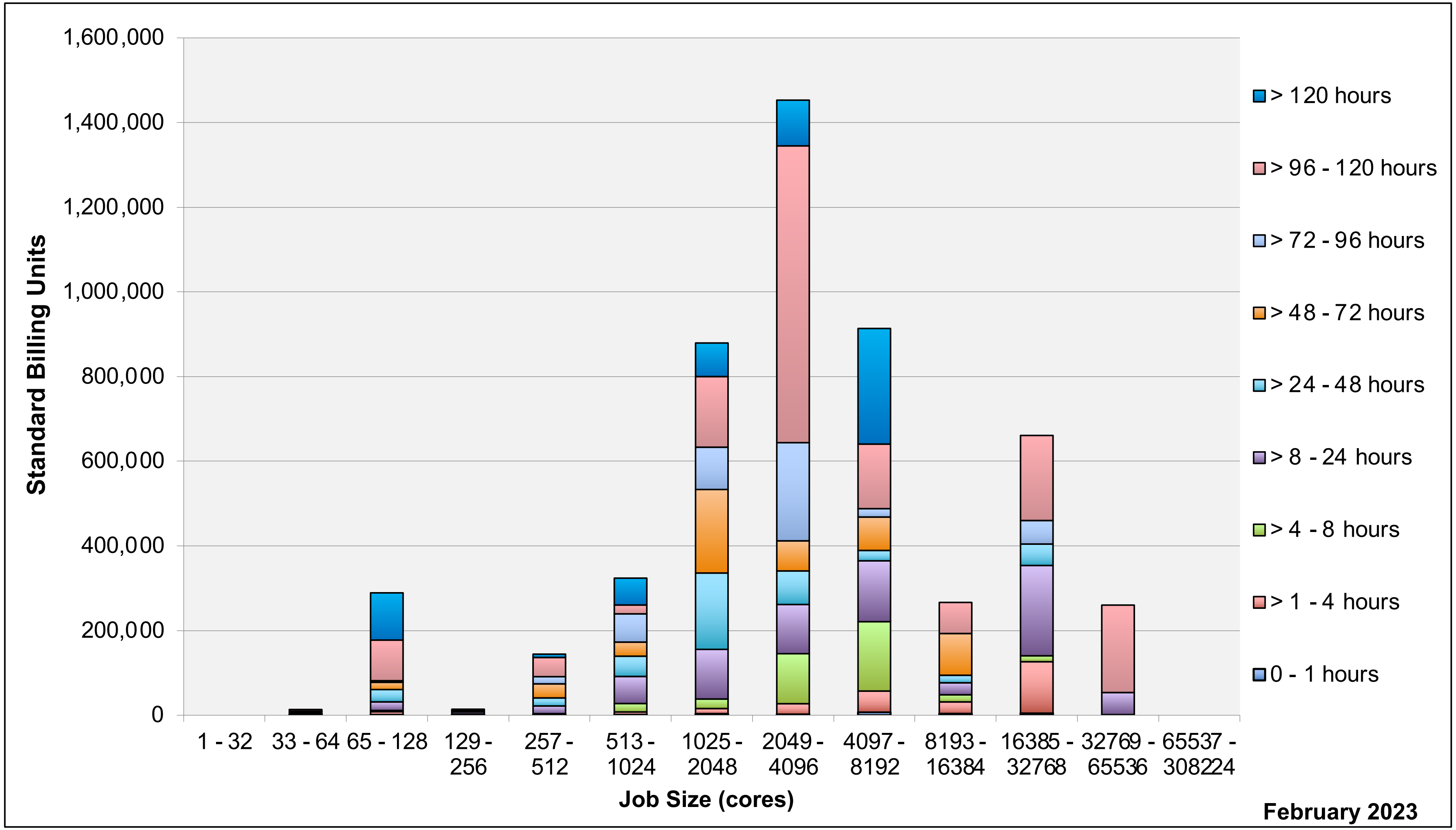
Aitken: Monthly Utilization by Job Length



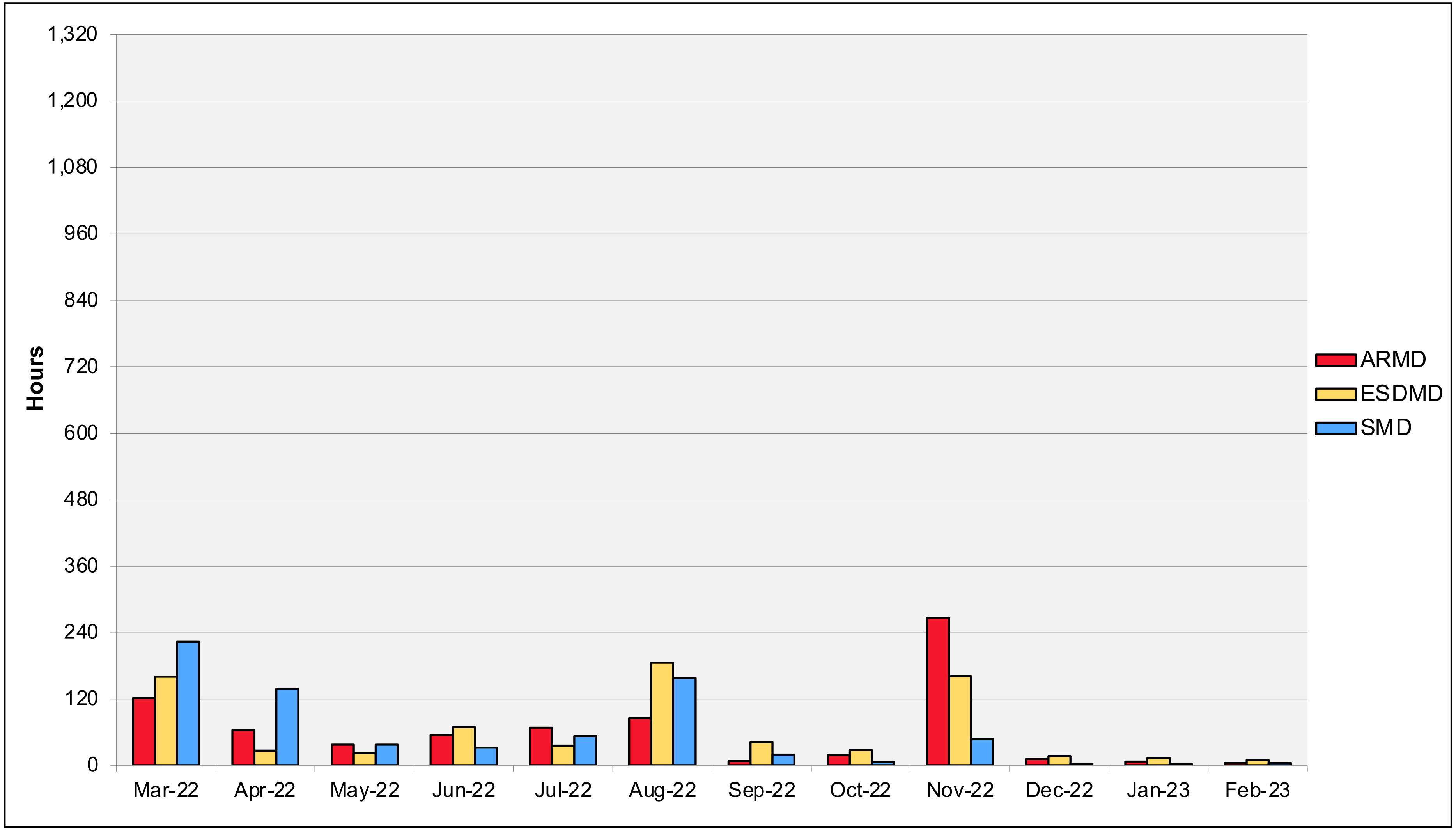
Aitken: Monthly Utilization by Job Size



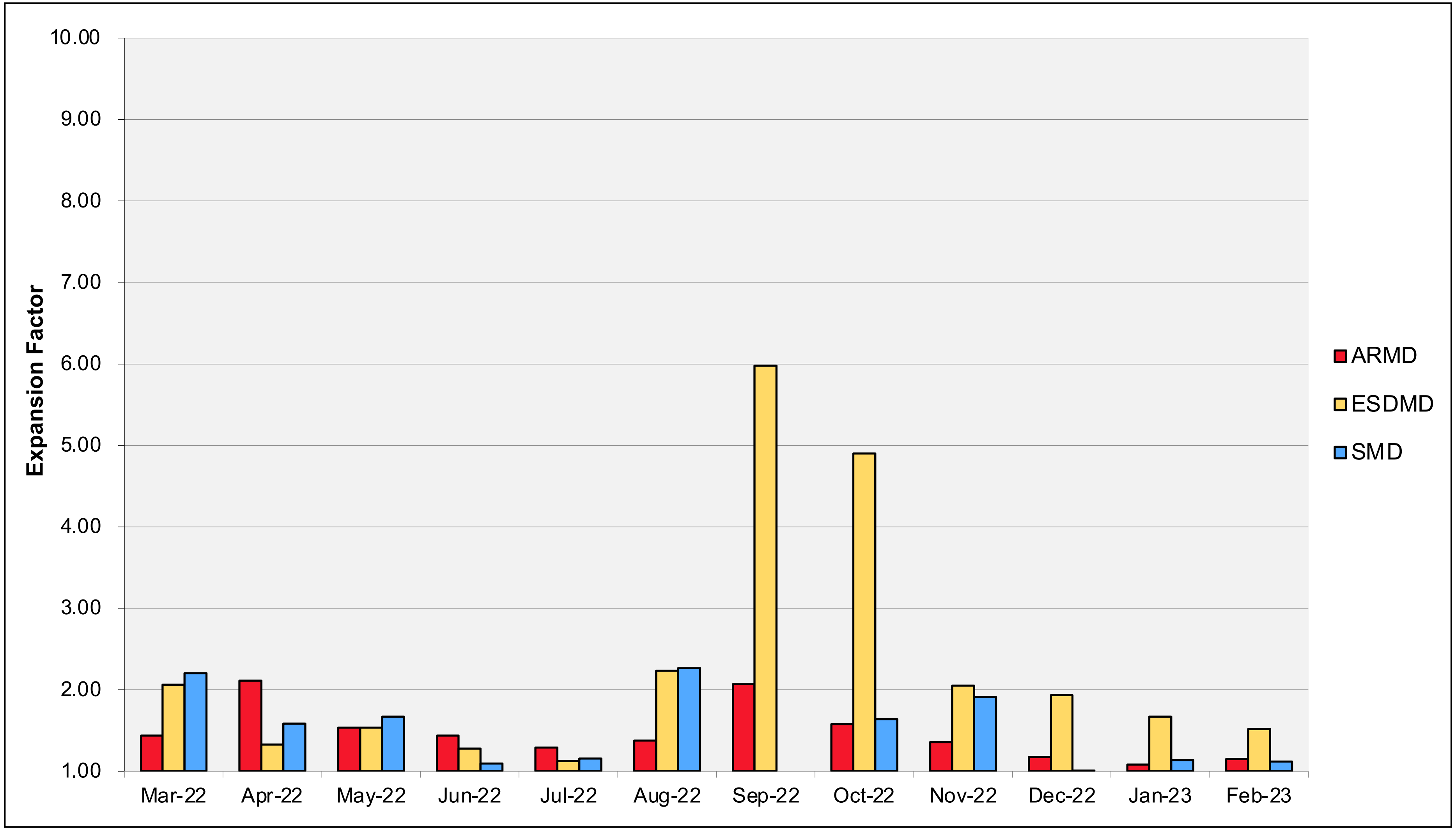
Aitken: Monthly Utilization by Size and Length



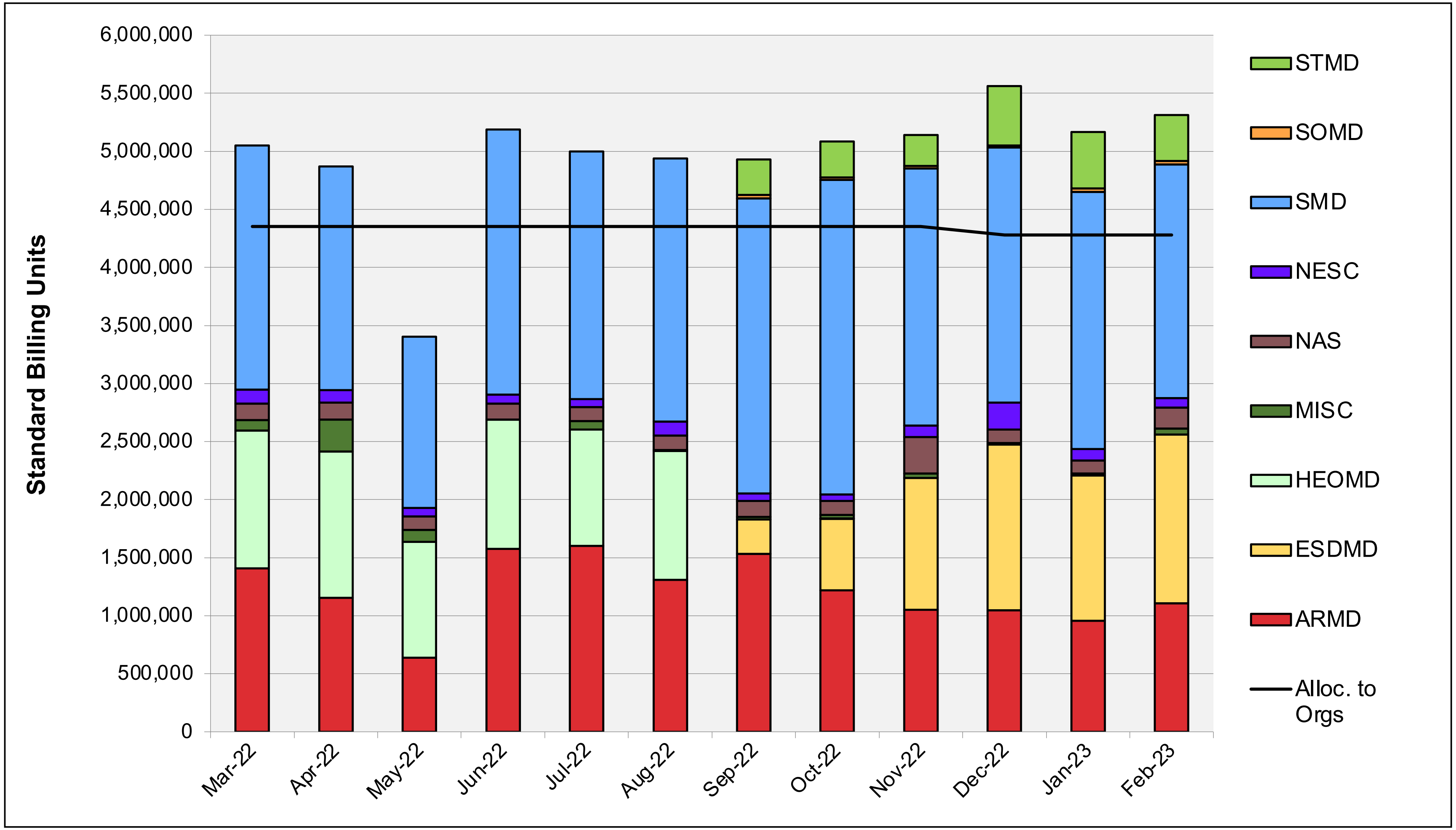
Aitken: Average Time to Clear All Jobs



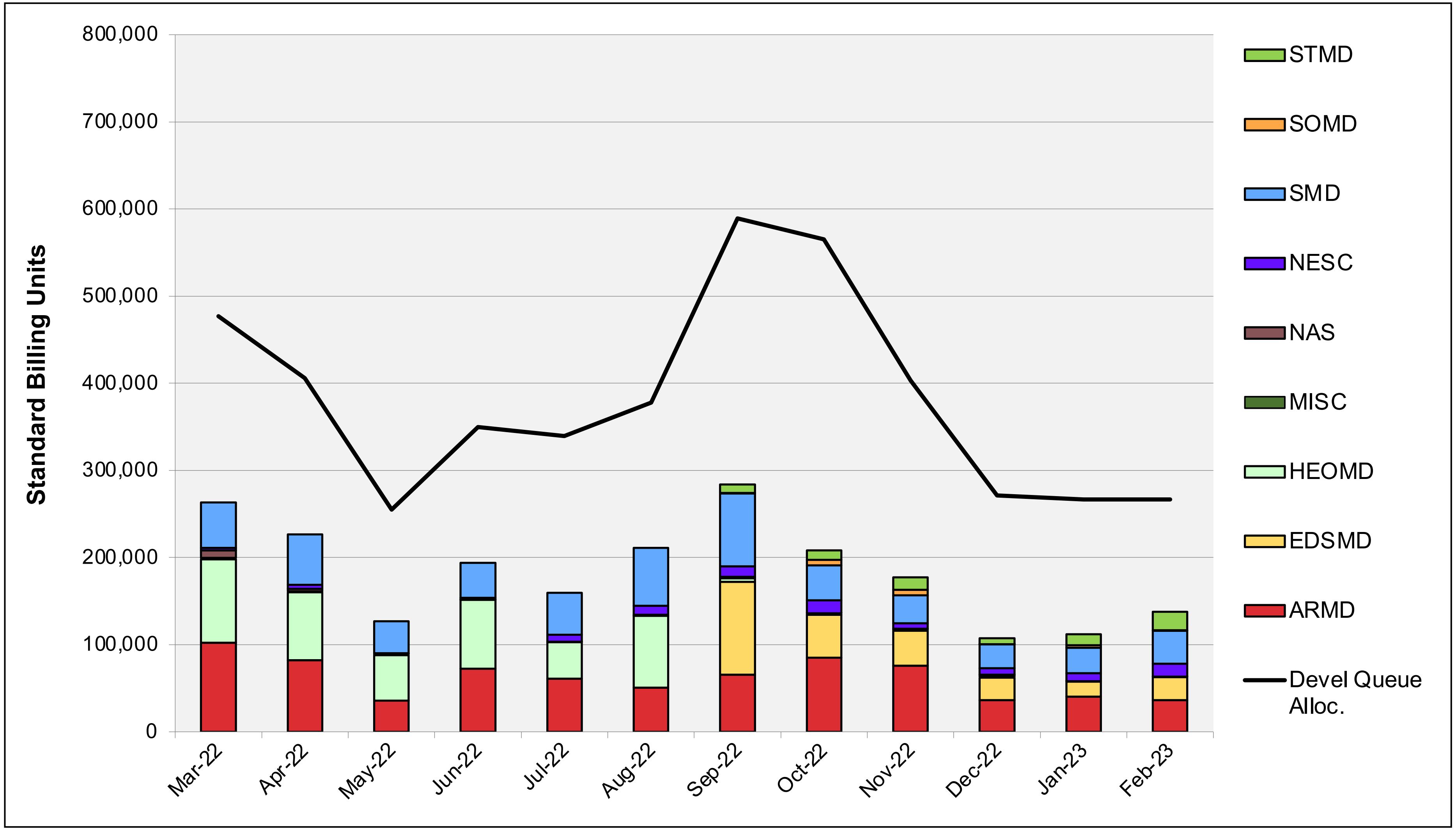
Aitken: Average Expansion Factor



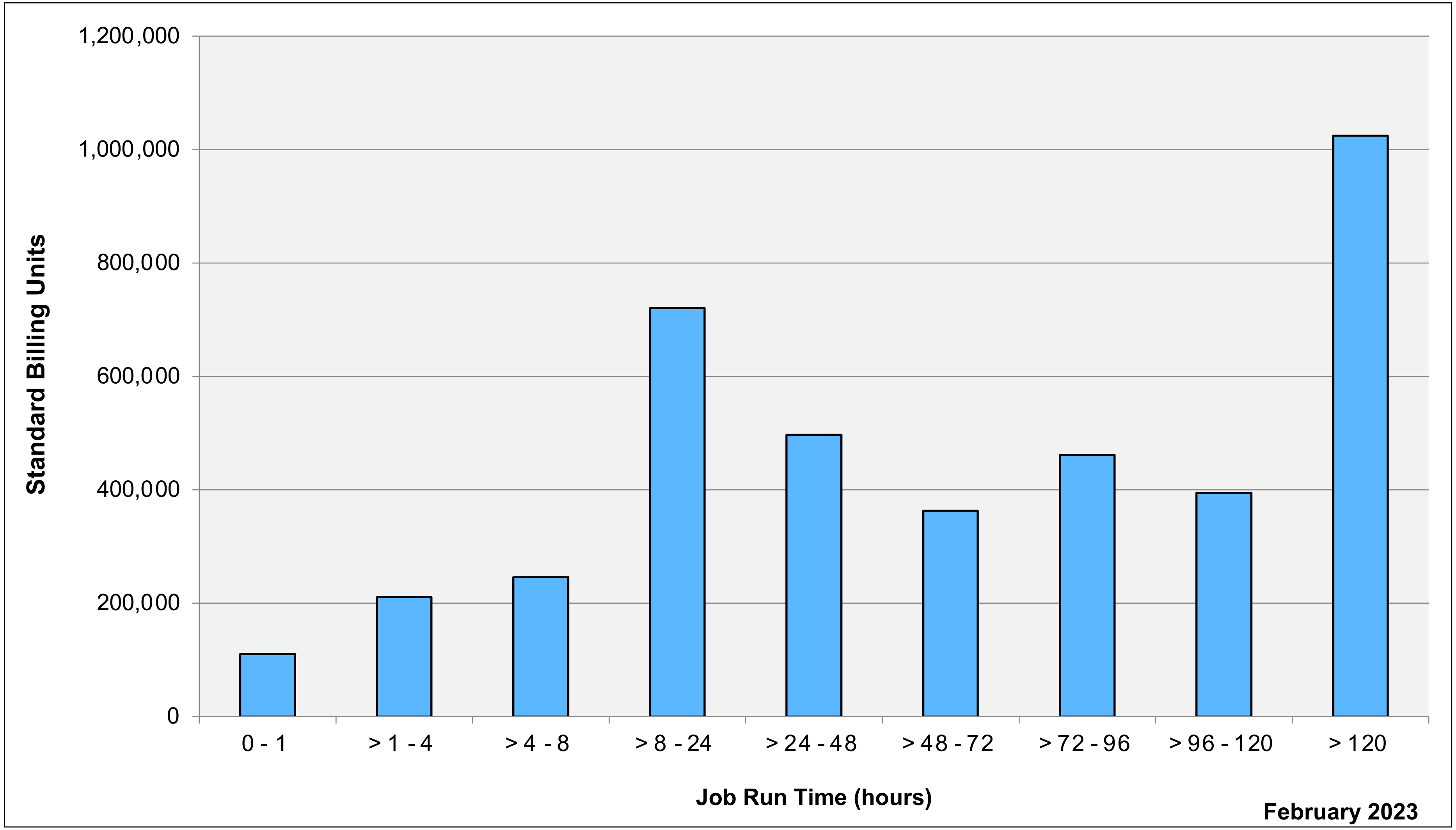
Pleiades: SBUs Reported, Normalized to 30-Day Month



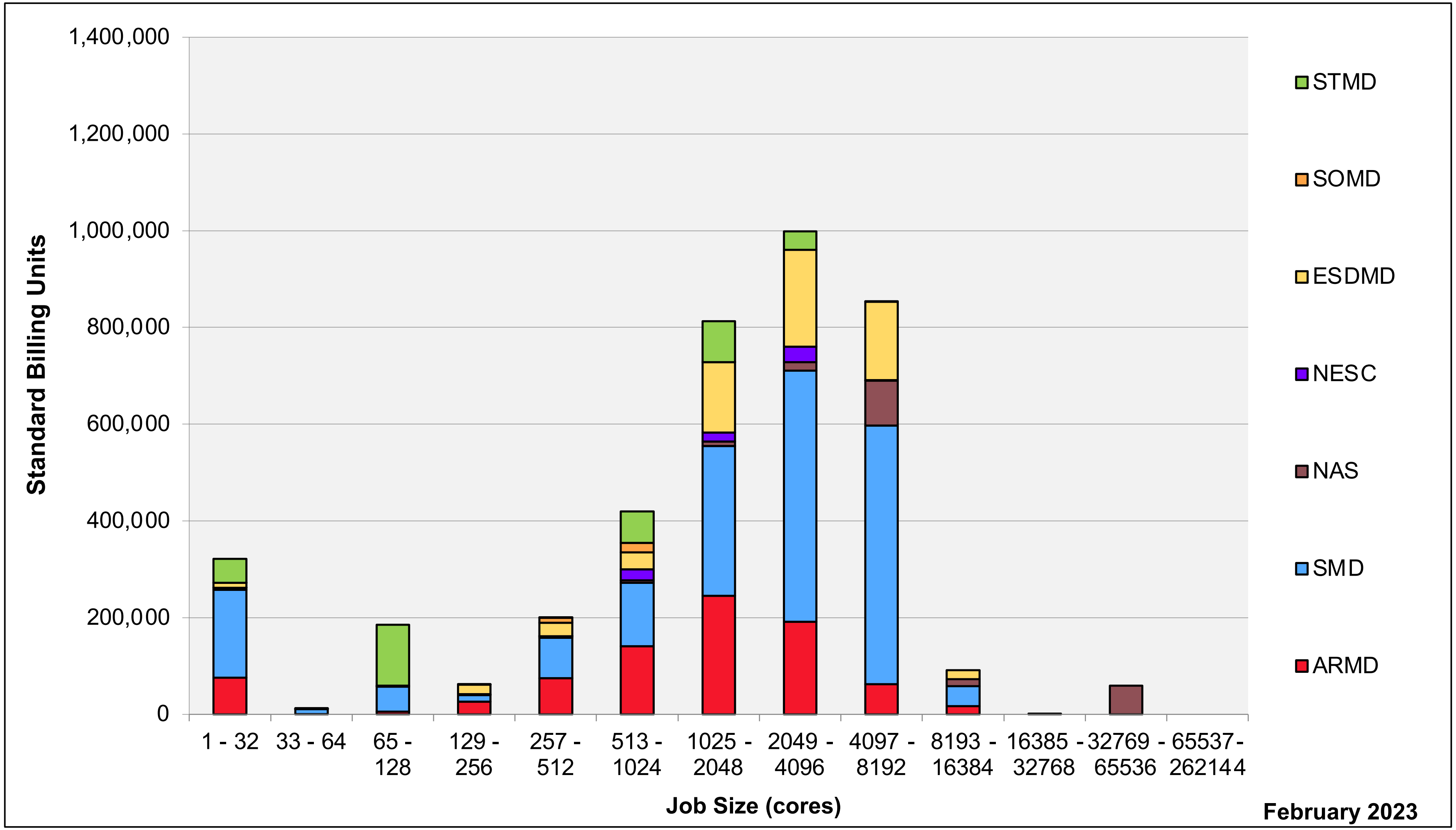
Pleiades: Devel Queue Utilization



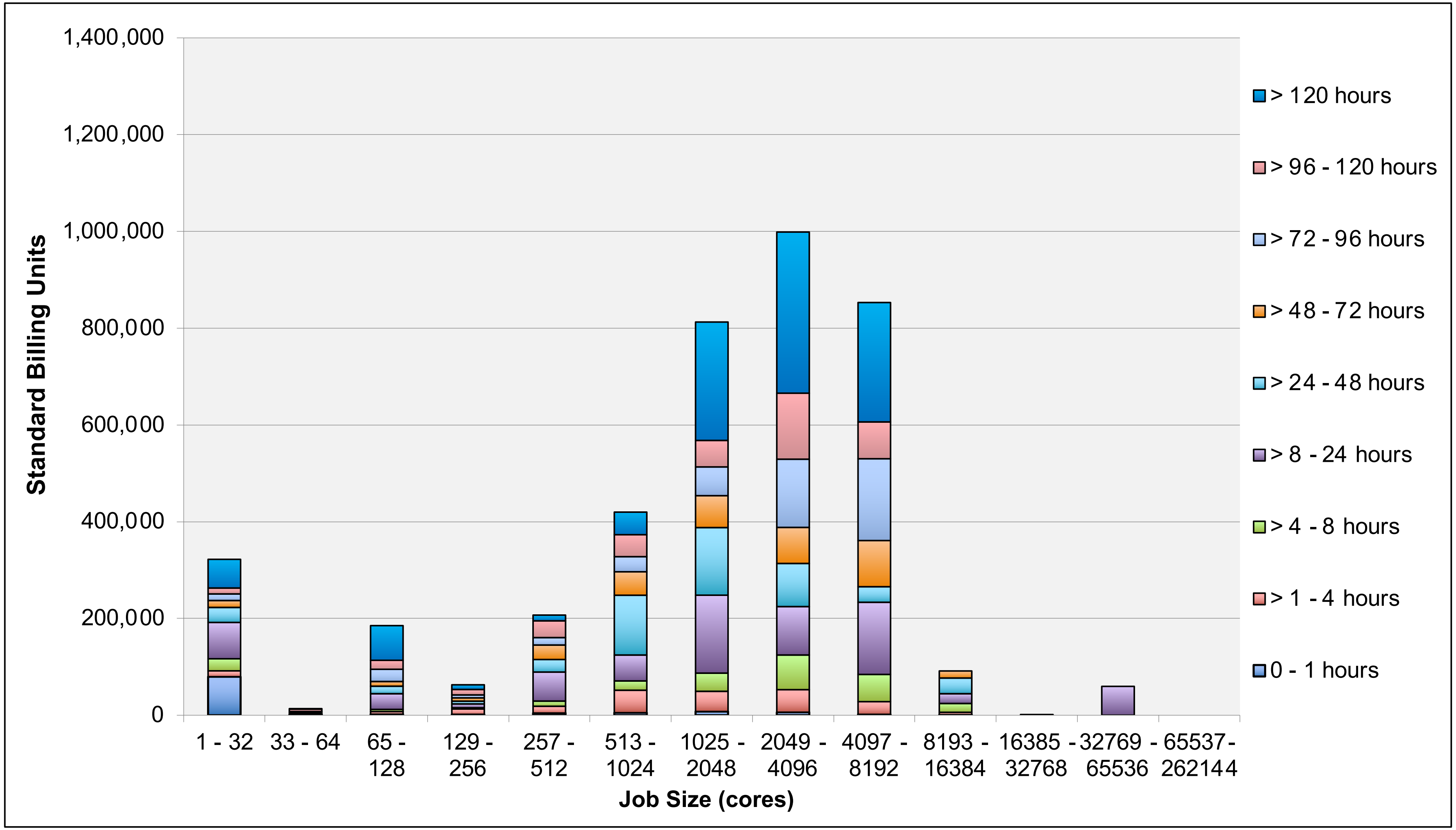
Pleiades: Monthly Utilization by Job Length



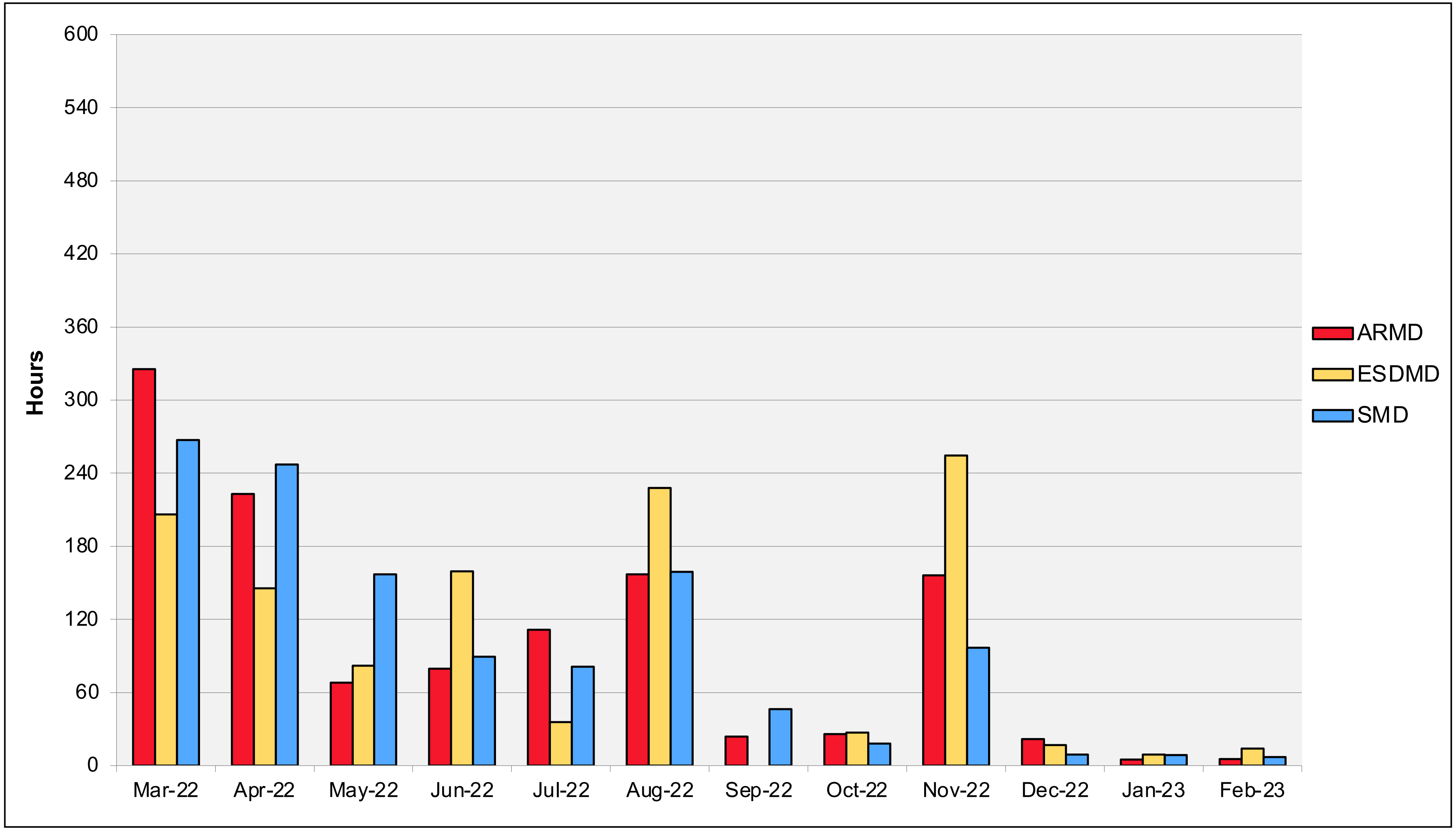
Pleiades: Monthly Utilization by Job Size



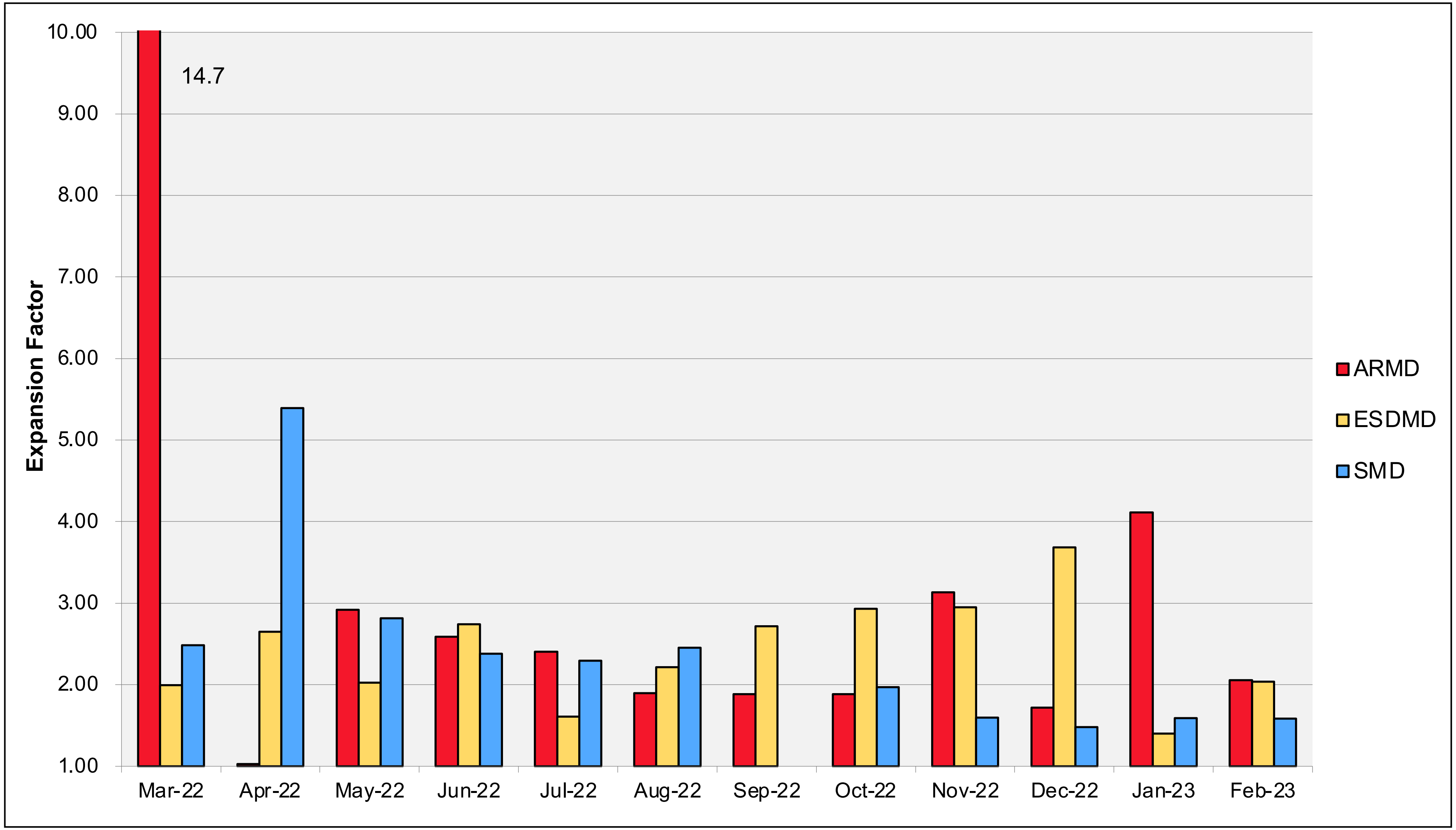
Pleiades: Monthly Utilization by Size and Length



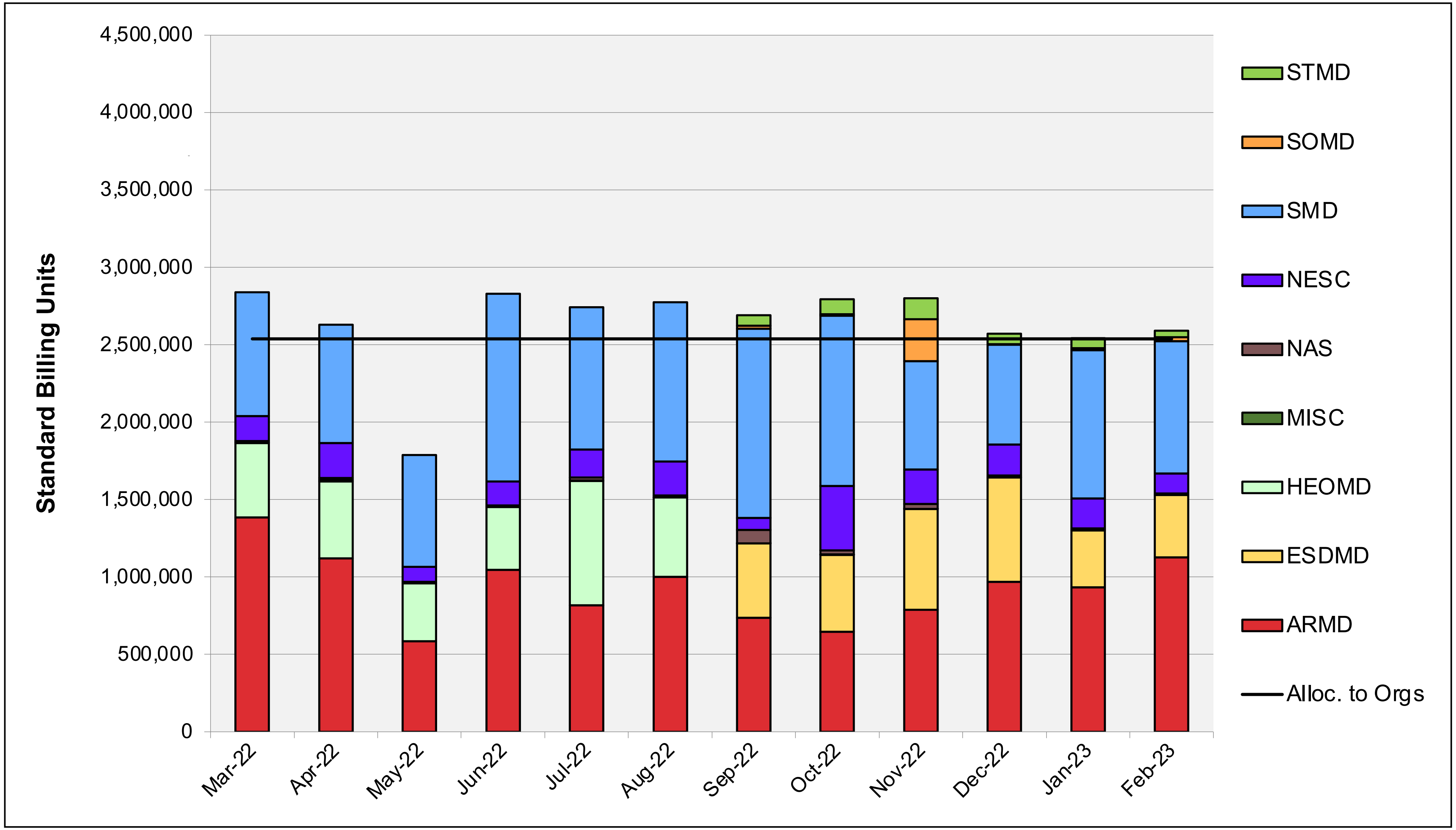
Pleiades: Average Time to Clear All Jobs



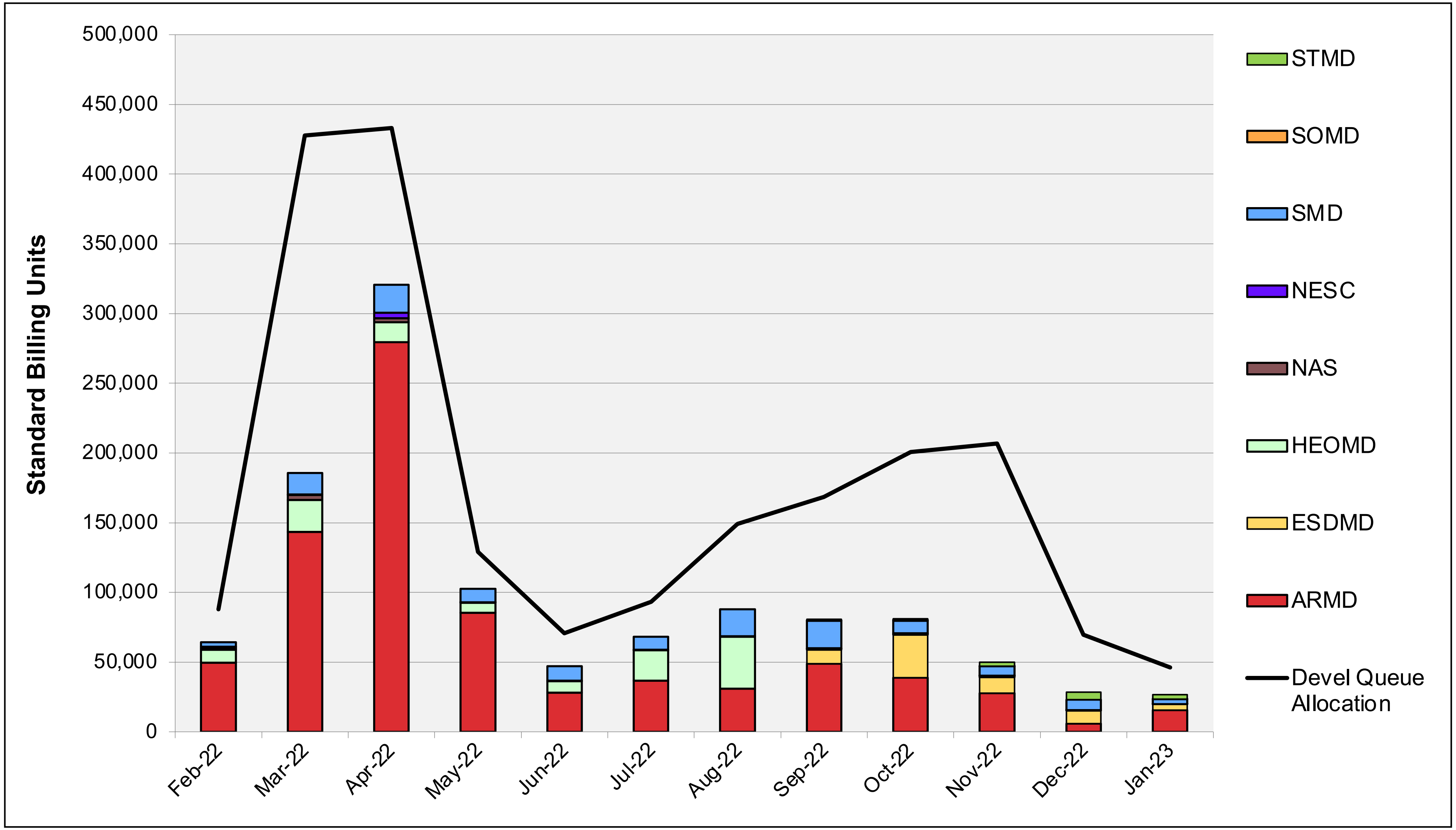
Pleiades: Average Expansion Factor



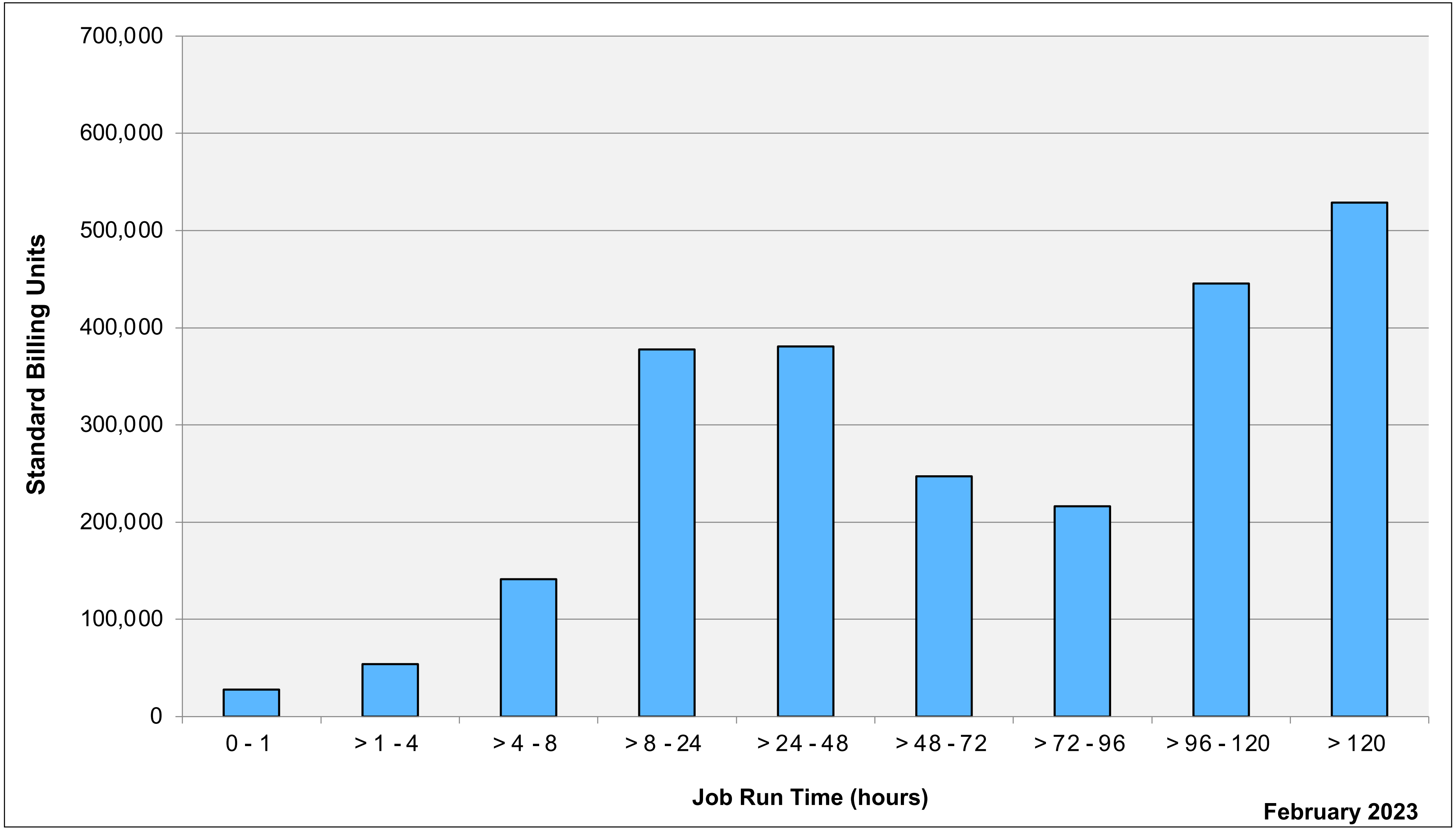
Electra: SBUs Reported, Normalized to 30-Day Month



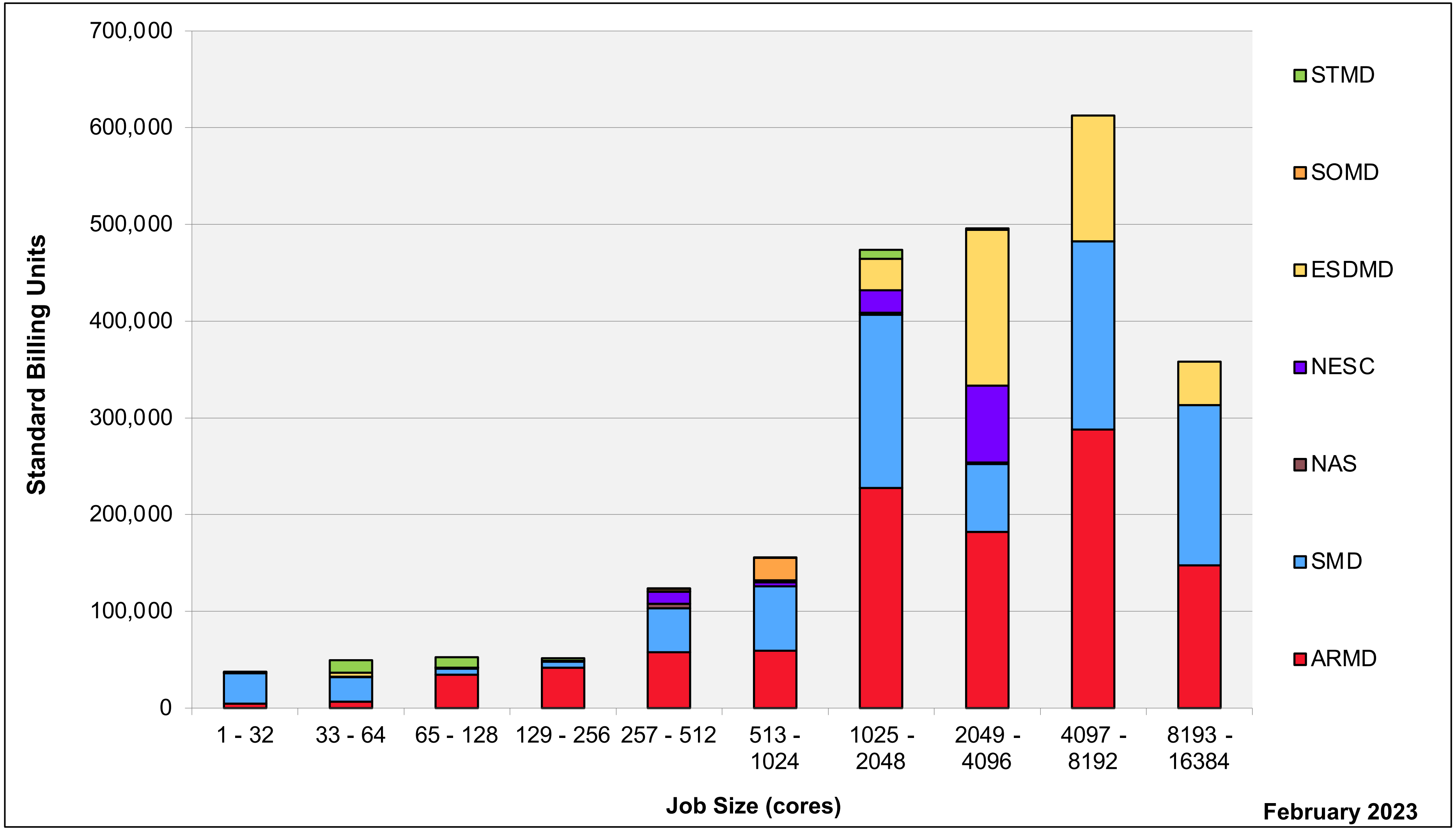
Electra: Devel Queue Utilization



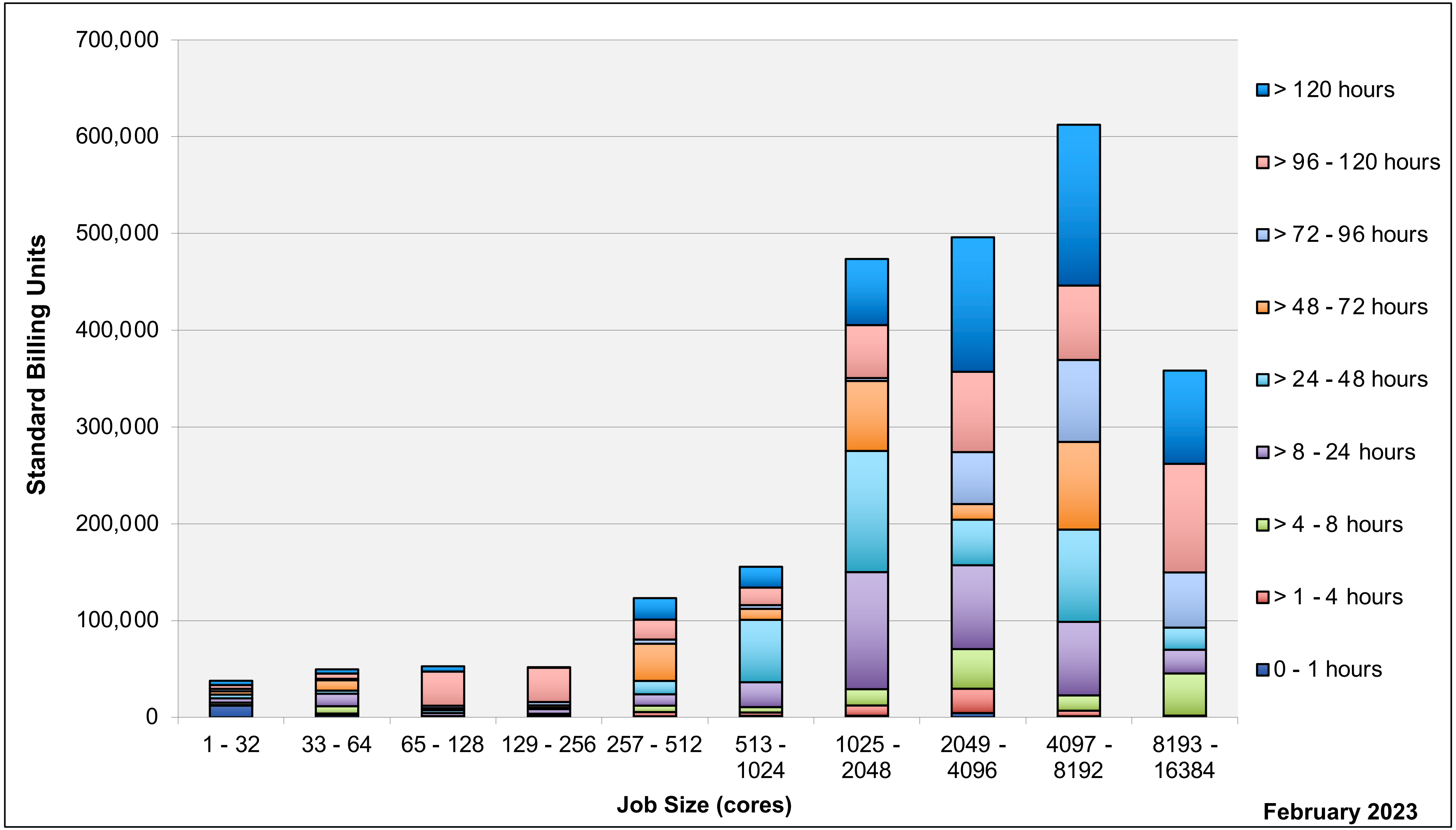
Electra: Monthly Utilization by Job Length



Electra: Monthly Utilization by Job Size



Electra: Monthly Utilization by Size and Length



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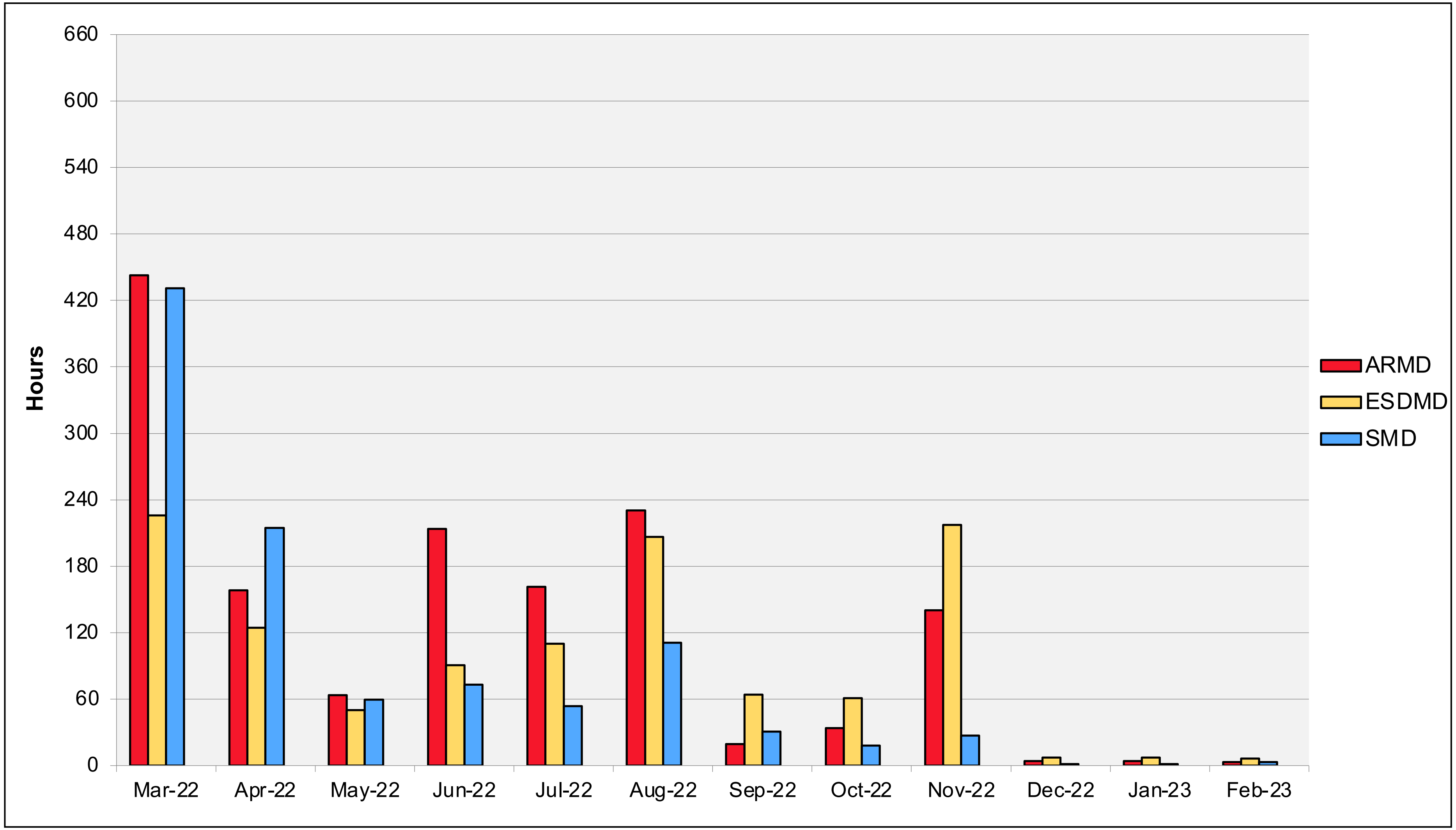

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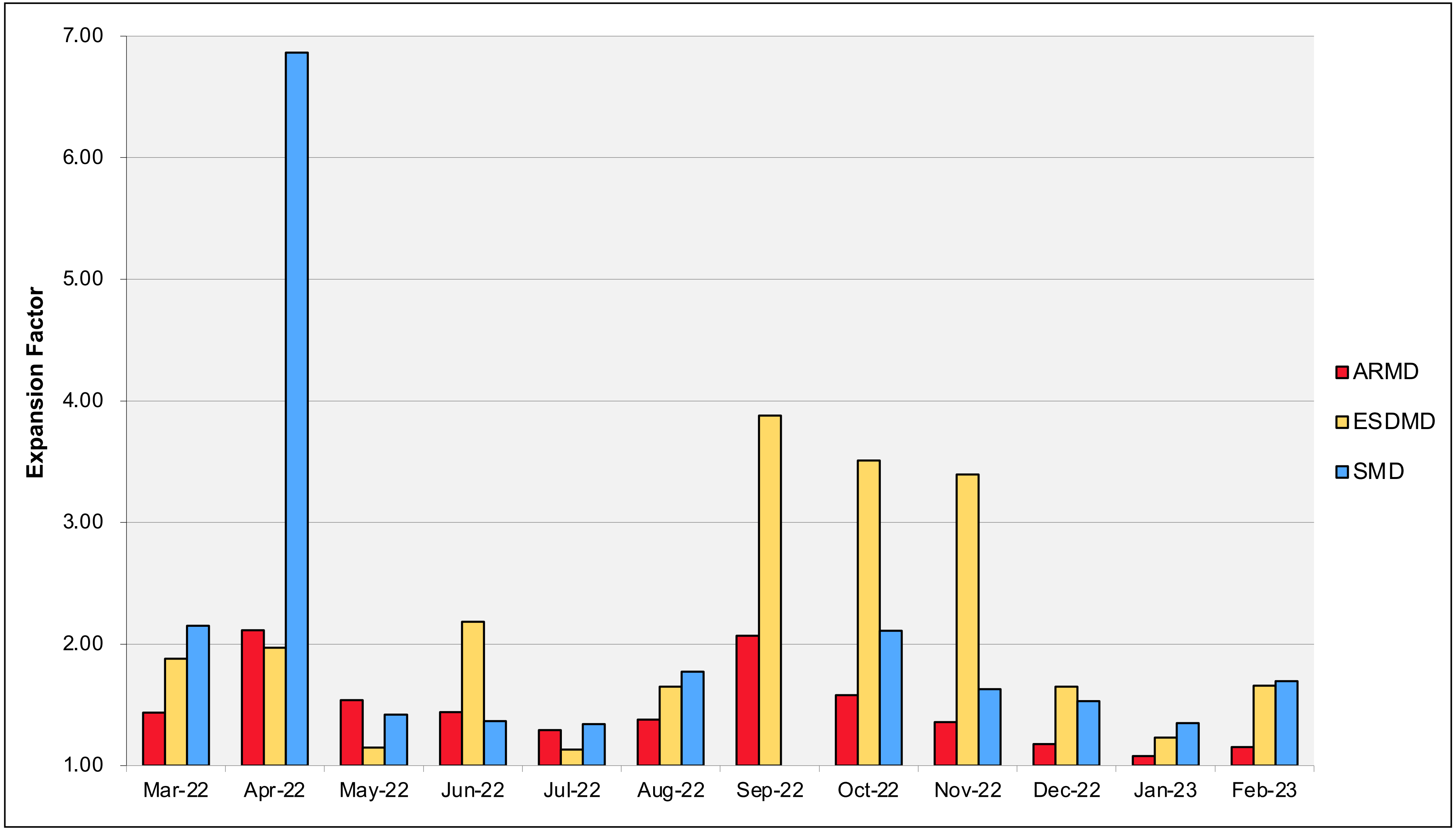
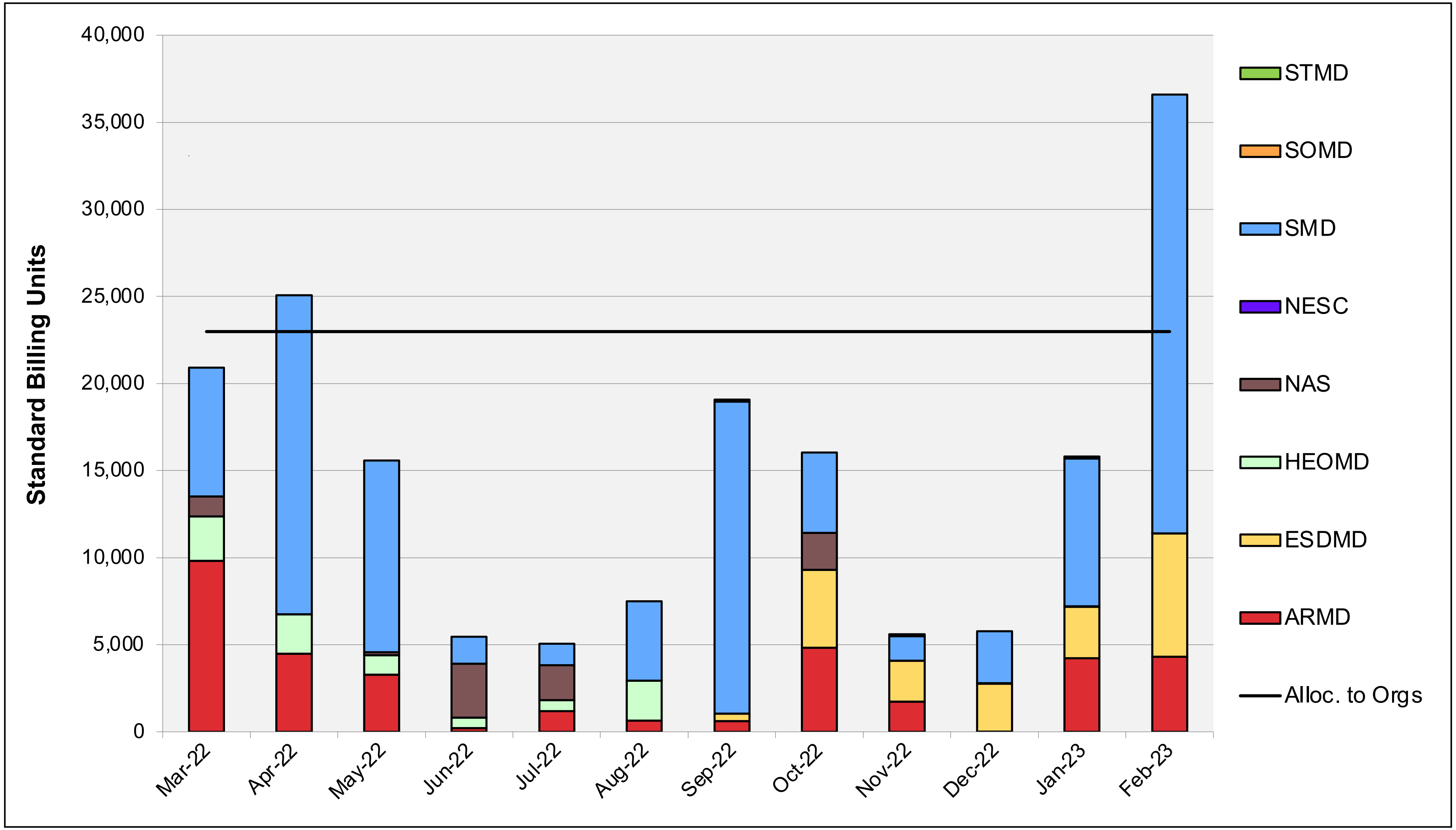
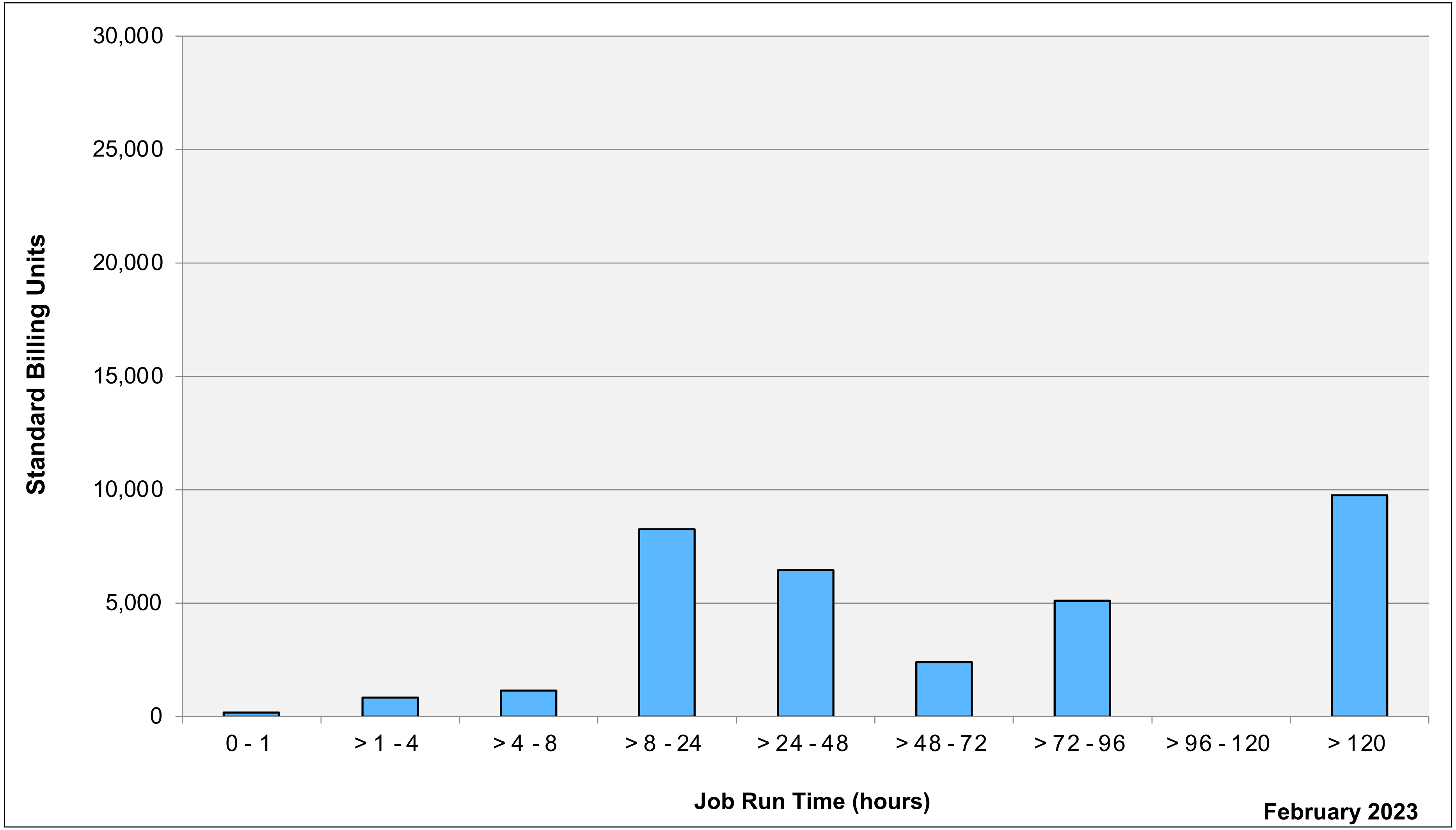


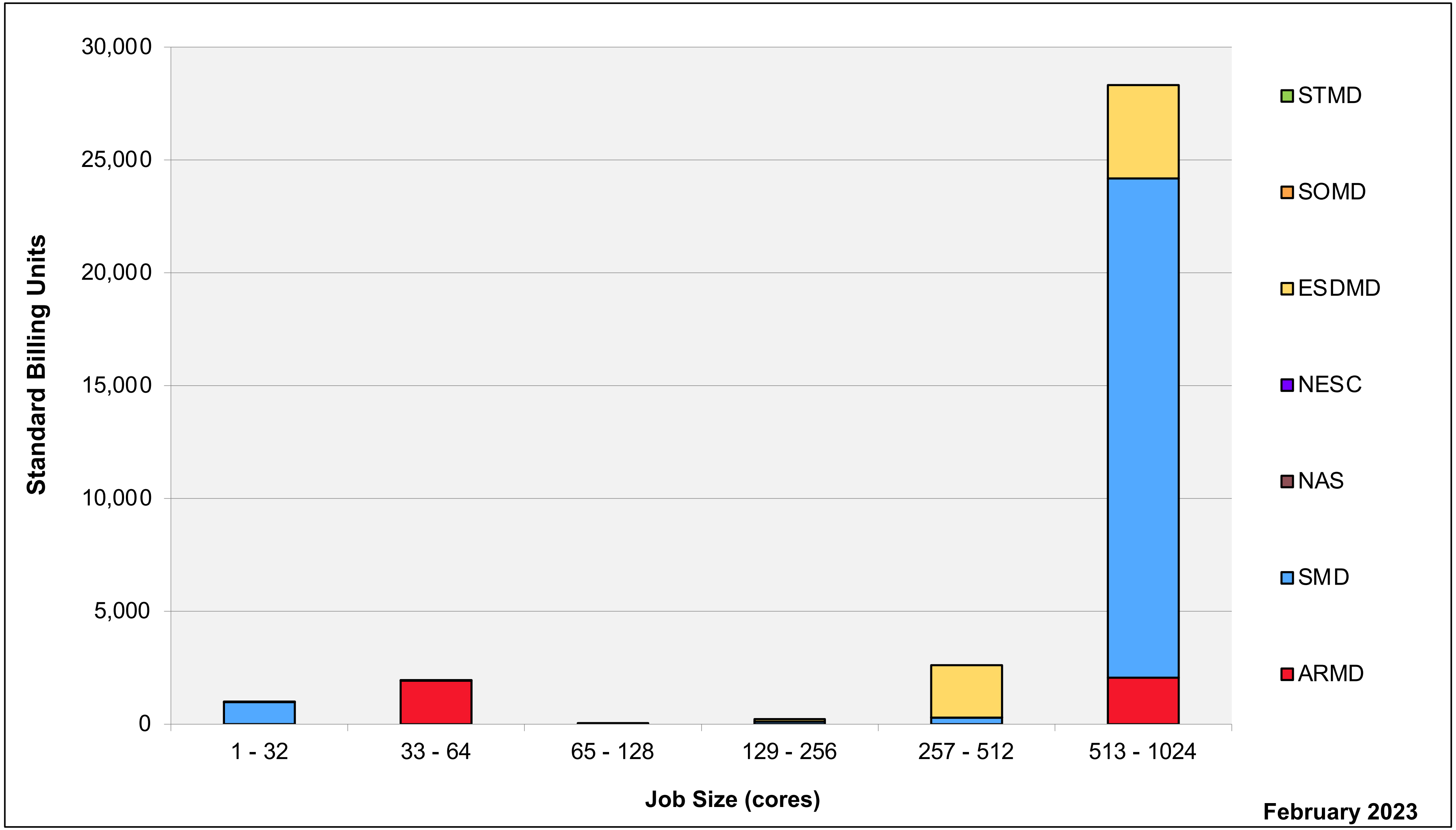
Endeavour: SBUs Reported, Normalized to 30-Day Month



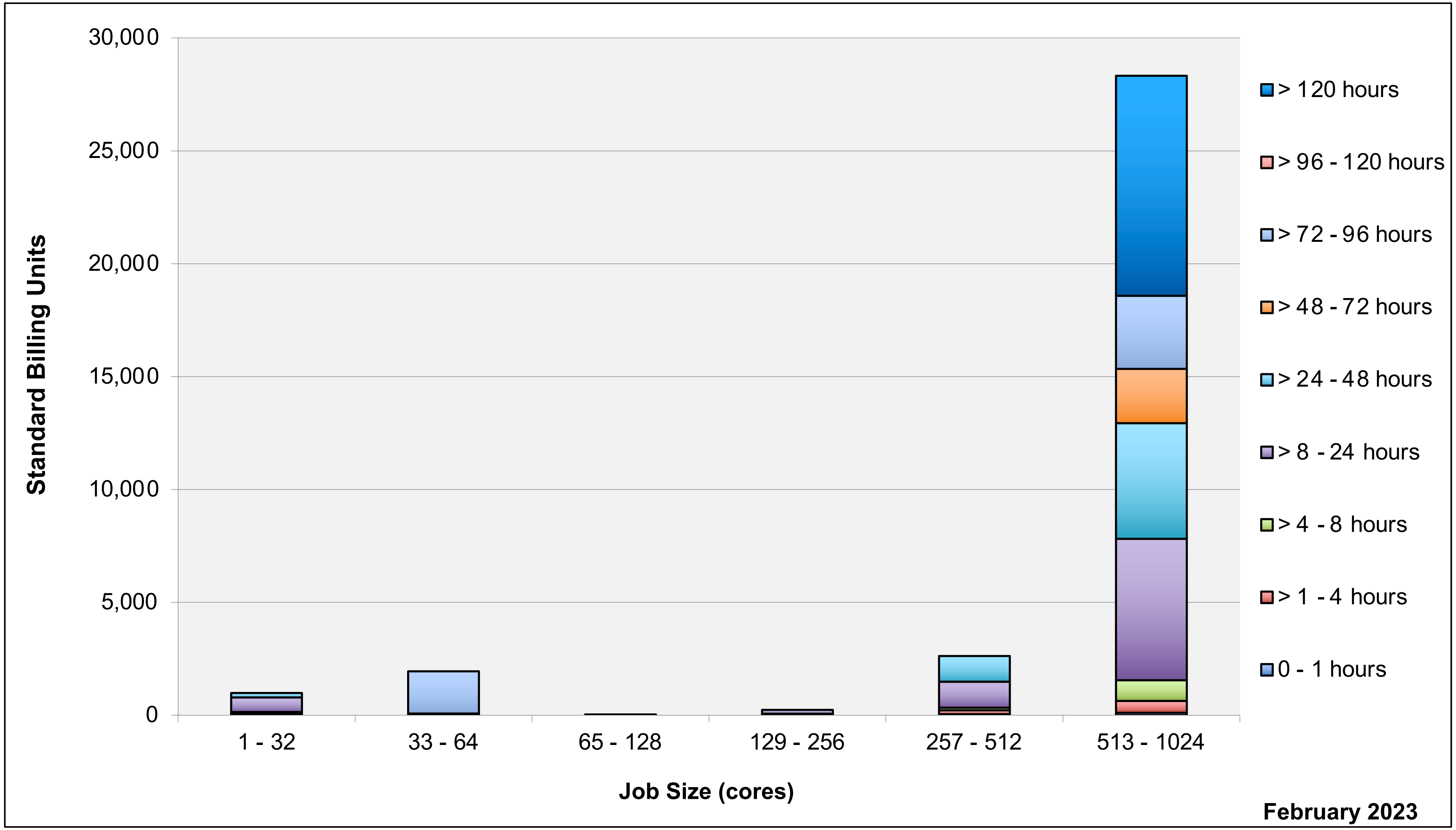
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor